

Supplementary Materials

A computational study of TyrGly hydration

Rabia Hameed and Tanja van Mourik

Figure S1: mPW2-PLYP/def2-TZVP structures of the singly hydrated Tyr-Gly conformers considered in this work

Table S1: Relative energies (in kJ/mol), hydrogen-bond distances ($R(\text{H}\cdots\text{O})$ in Å) and hydrogen-bond angles ($\angle\text{OH}\cdots\text{O}$ in degrees) for conformers with an $\text{OH}\cdots\text{O}$ hydrogen bond and R_{CC} distances (in Å) for the optimised monohydrated clusters. See caption of Figure 4 in the main text for an explanation of the labels

Table S2: Cartesian coordinates (in Å) of the gas-phase, implicitly solvated and monohydrated structures optimised with mPW2PLYP-D2/def2-TZVP in xyz format. The title line indicates the phase (gas, implicit solvation, explicit solvation), conformer number and, for the monohydrated structures, the starting position of the

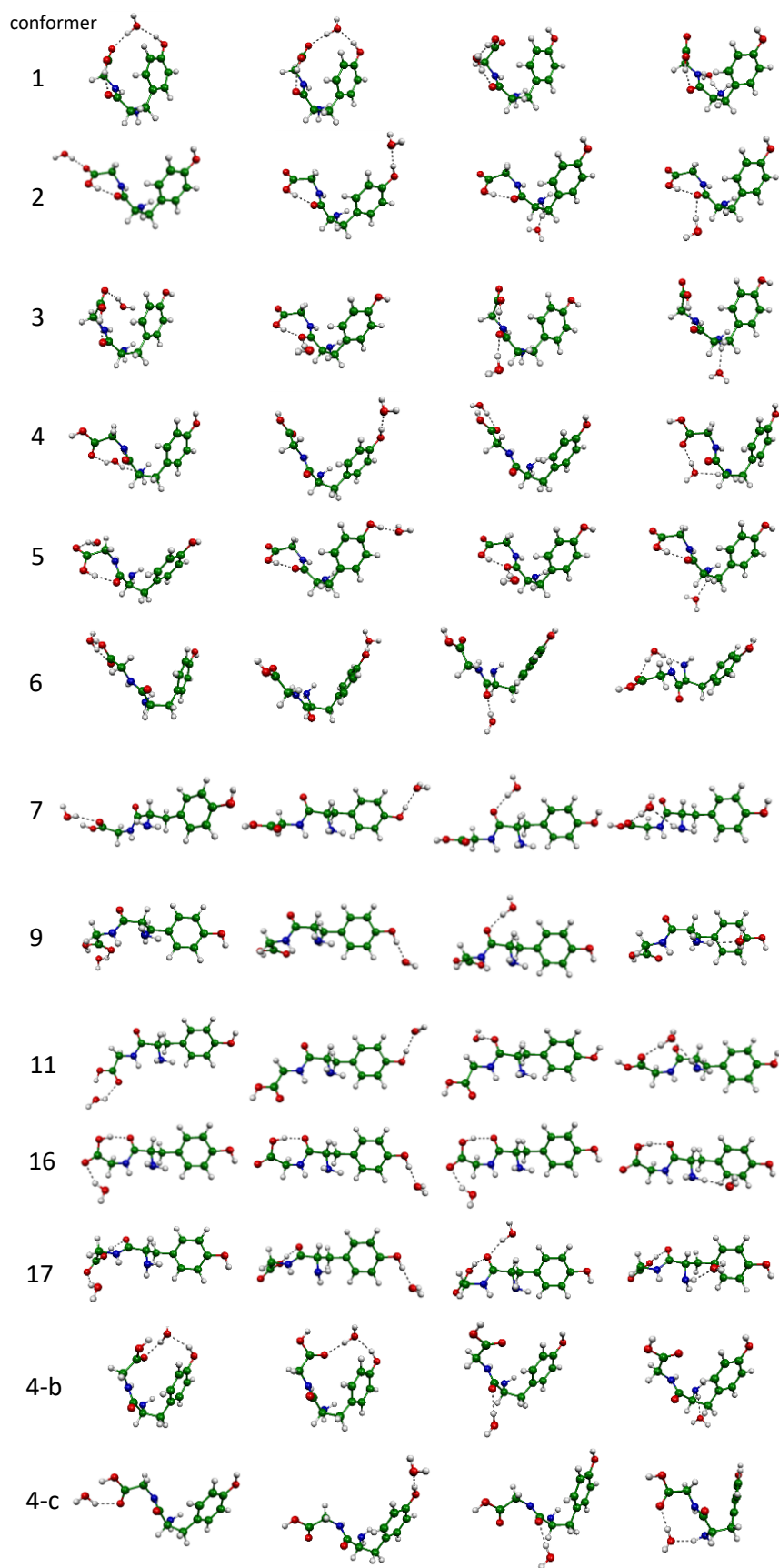


Figure S1. mPW2-PLYP/def2-TZVP structures of the singly hydrated Tyr-Gly conformers considered in this work

Table S1. Relative energies (in kJ/mol), hydrogen-bond distances ($R(\text{H}\cdots\text{O})$ in Å) and hydrogen-bond angles ($\angle\text{OH}\cdots\text{O}$ in degrees) for conformers with an $\text{OH}\cdots\text{O}$ hydrogen bond and R_{CC} distances (in Å) for the optimised monohydrated clusters. See caption of Figure 4 in the main text for an explanation of the labels

Conf.	ΔE	$R(\text{H}\cdots\text{O})$	$\angle\text{OH}\cdots\text{O}$	R_{CC}	Conf.	ΔE	$R(\text{H}\cdots\text{O})$	$\angle\text{OH}\cdots\text{O}$	R_{CC}
1_CO	27.04	159	1.74	5.29	6_CO	32.81			6.37
1_COcarb	1.99	158	1.70	4.35	6_COcarb	21.28			6.80
1_NH	28.35	159	1.71	5.40	6_NH	36.01			6.81
1_NH2-1	38.50	160	1.70	5.51	6_NH2-1	31.08			7.55
1_NH2-2	21.01	153	1.74	4.55	6_NH2-2	22.77			5.81
1_OH	0.00	158	1.70	4.32	6_OH	36.18			6.80
1_OHcarbH	15.17			4.52	6_OHcarbH	21.27			6.79
1_OHcarbO	12.23	160	1.72	4.41	6_OHcarbO	50.51			7.81
2_CO	32.04	161	1.74	7.28	7_CO	27.17			9.50
2_COcarb	40.39	162	1.70	7.44	7_COcarb	28.47			9.56
2_NH	24.80	157	1.75	7.50	7_NH	30.62			9.17
2_NH2-1	41.13	162	1.72	7.50	7_NH2-1	28.47			9.56
2_NH2-2	33.86	162	1.73	7.27	7_NH2-2	47.73			9.50
2_OH	28.52	162	1.72	7.43	7_OH	37.25			9.48
2_OHcarbO	37.41	162	1.69	7.44	7_OHcarbH	23.10			9.46
3_CO	30.33	160	1.73	5.59	7_OHcarbO	51.44			9.45
3_COcarb	24.93	155	1.72	4.94	9_CO	28.21			8.82
3_NH	31.67	159	1.72	5.80	9_COcarb	23.95			8.73
3_NH2-1	42.06	161	1.70	5.74	9_NH	31.19			8.65
3_NH2-2	24.91	155	1.72	4.92	9_NH2-1	46.85			8.57
3_OH	29.33	161	1.71	5.75	9_NH2-2	44.92			8.56
3_OHcarbO	30.75	159	1.66	5.60	9_OH	37.43			8.73
4_CO	27.06	159	1.74	5.30	9_OHcarbH	24.82			8.72
4_COcarb	30.48			7.58	9_OHcarbO	50.86			8.73
4_NH	28.37	159	1.71	5.40	11_CO	34.68			9.53
4_NH2-1	38.72			6.44	11_COcarb	28.47			9.56
4_NH2-2	20.98	153	1.74	4.55	11_NH	31.05			9.24
4_OH	35.74			6.85	11_NH2-1	28.48			9.56
4_OHcarbH	20.44			6.94	11_NH2-2	47.87			9.51
4_OHcarbO	0.05	158	1.70	4.32	11_OH	37.68			9.54
5_CO	34.87	161	1.76	7.30	11_OHcarbH	23.55			9.54
5_COcarb	25.45	157	1.75	7.49	11_OHcarbO	51.44			9.46
5_NH	25.45	157	1.75	7.48	16_CO	27.60	160	1.76	9.64
5_NH2-1	41.87	161	1.72	7.50	16_COcarb	27.09	157	1.75	9.56
5_NH2-2	37.70	161	1.73	7.76	16_NH	27.19	157	1.75	9.56
5_OH	29.51	161	1.73	7.46	16_NH2-1	42.60	161	1.73	9.68
5_OHcarbO	38.32	161	1.69	7.46	16_NH2-2	32.46	155	1.73	9.43
					16_OH	31.59	161	1.73	9.65
					16_OHcarbH	23.86			9.58
					16_OHcarbO	32.45	155	1.73	9.43

Table S1. Continued

Conf.	ΔE	$R(H\cdots O)$	$\angle OH\cdots O$	R_{CC}	Conf.	ΔE	$R(H\cdots O)$	$\angle OH\cdots O$	R_{CC}
17_CO	27.69	160	1.76	9.19	4b_CO	32.89			5.72
17_COcarb	31.82	156	1.75	9.36	4b_COcarb	11.62			4.17
17_Cocarb 2	30.88	156	1.75	9.36	4b_OHcarbH	21.64			5.90
17_NH	37.10	160	1.74	9.57	4b_NH	34.09			5.87
17_NH2-1	37.17	161	1.73	9.50	4b_NH2-1	50.08			5.78
17_NH2-2	114.39	158	1.65	8.90	4b_NH2-2	21.88			5.69
17_OH	35.47	161	1.73	9.51	4b_OH	25.96			5.09
17_OHcarbO	31.81	157	1.71	9.30	4b_OHcarbH	11.56			4.17
4c_CO	34.69			7.58	4b_OHcarbO	36.82			5.80
4c_COcarb	28.94			6.45					
4c_NH	30.48			7.58					
4c_NH2-1	28.82			6.47					
4c_NH2-2	39.93			7.87					
4c_OH	36.77			7.83					
4c_OHcarbH	21.26			7.82					
4c_OHcarbO	49.81			7.80					

Table S2. Cartesian coordinates (in Å) of the gas-phase, implicitly solvated and monohydrated structures optimised with mPW2PLYP-D2/def2-TZVP in xyz format. The title line indicates the phase (gas, implicit solvation, explicit solvation), conformer number and, for the monohydrated structures, the starting position of the water molecule (see caption of Figure 4 in the main document for the labelling)

31			
gasphase-1.xyz			
N	-0.12697800	-2.44633600	-1.40670600
C	-0.48856200	-2.37619600	0.00473400
C	-1.53365900	-1.29443400	0.25609000
N	-1.93840500	-0.60793000	-0.81413300
O	-1.95703700	-1.07316300	1.39566100
H	0.01939900	-3.39923000	-1.70253500
C	0.70801400	-2.16139200	0.95747400
C	1.51111000	-0.94546400	0.58840800
C	1.08639400	0.33214800	0.95153100
C	1.77408100	1.46233000	0.53845900
C	2.91558100	1.33353200	-0.24636100
C	3.36726400	0.06936300	-0.60464500
C	2.66459300	-1.05231000	-0.18852900
O	3.63048500	2.40559300	-0.68286100
H	-0.98009200	-3.30907400	0.28522700
H	0.31962000	-2.07759600	1.97082900
H	1.33643900	-3.05100500	0.90879700
H	0.20648000	0.45233800	1.56534500
H	1.41868000	2.44362900	0.82582900
H	4.26349700	-0.01922300	-1.20067600
H	3.03005900	-2.03335800	-0.46388500
H	3.20754300	3.21622800	-0.38374600
H	0.72398500	-1.92659100	-1.58470200
C	-2.98024900	0.39994800	-0.75825200
C	-2.53066500	1.69764000	-0.08473700
O	-2.16036100	1.57157800	1.19059300
O	-2.53094600	2.75476900	-0.65275200
H	-1.54153000	-0.90060400	-1.69509800
H	-3.83493400	0.00236900	-0.20729400
H	-3.28491100	0.64053200	-1.77005200
H	-2.20324000	0.62199000	1.45972400
31			
gasphase-2.xyz			
N	0.12636900	2.07953900	-1.39686000
C	0.41998900	1.93365100	0.02352000
C	1.26846600	0.69349400	0.28317800
N	1.72462800	0.05726800	-0.79796200
O	1.52913400	0.32798800	1.43401200
H	0.03511100	3.05172100	-1.65149900
C	-0.81532100	1.92329600	0.94622100
C	-1.80017100	0.85024100	0.57625200
C	-1.63531600	-0.46126800	1.02078100
C	-2.51630800	-1.46245400	0.63898800
C	-3.58555000	-1.16800400	-0.20100500
C	-3.77118200	0.13354200	-0.64959000
C	-2.88356300	1.12496100	-0.25846600
O	-4.48187300	-2.10817200	-0.60724900
H	1.05418400	2.77028400	0.32300000
H	-0.47005600	1.79062100	1.96965800
H	-1.28993300	2.90231700	0.87480100
H	-0.80936400	-0.69768800	1.67656300

H	-2.37774600	-2.47369200	1.00051300
H	-4.61315400	0.35411900	-1.28888300
H	-3.04812600	2.13990900	-0.59650600
H	-4.25576700	-2.95820900	-0.21824200
H	-0.74245600	1.61319600	-1.62966000
C	2.46814500	-1.18552800	-0.72470600
C	3.91147500	-1.02544800	-0.24554400
O	4.05330100	-0.45422500	0.94979400
O	4.84663200	-1.41224300	-0.89081100
H	1.50547100	0.48554100	-1.68536400
H	2.49544300	-1.63328700	-1.71134900
H	1.95450700	-1.86086200	-0.03762800
H	3.17121800	-0.22085300	1.32275200

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gasphase-3.xyz

N	-0.11470300	-2.40374900	-1.40602100
C	-0.46841300	-2.34248300	0.00780600
C	-1.53179000	-1.28070700	0.26837400
N	-1.99185600	-0.63241200	-0.80346100
O	-1.92878400	-1.04872900	1.41492900
H	0.06707800	-3.35193300	-1.69798500
C	0.72841900	-2.12245800	0.95701000
C	1.54337900	-0.91713900	0.57927600
C	2.71281900	-1.04927900	-0.16359700
C	3.44248600	0.06239200	-0.56932200
C	3.00122100	1.33616700	-0.23428800
C	1.83603800	1.48997000	0.51115200
C	1.12309600	0.37388700	0.91179300
O	3.66716500	2.46520100	-0.59889200
H	-0.94739100	-3.28323700	0.28481100
H	0.34017100	-2.02676600	1.96942500
H	1.35241000	-3.01574700	0.91852800
H	3.07331400	-2.03738000	-0.41893800
H	4.35509600	-0.06289100	-1.13817300
H	1.50257900	2.48403300	0.76956800
H	0.22612300	0.51075900	1.49768800
H	4.45285200	2.22886900	-1.10055200
H	0.71679600	-1.85449700	-1.58849200
C	-3.08250300	0.32246600	-0.73970400
C	-2.69001300	1.65930000	-0.10866100
O	-2.24814600	1.58265700	1.14760800
O	-2.79588900	2.70234600	-0.69198100
H	-1.60902000	-0.92809600	-1.68949000
H	-3.89944800	-0.10621600	-0.15555100
H	-3.42798500	0.52211900	-1.74728800
H	-2.23070300	0.64012800	1.44070800

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gasphase-4.xyz

N	0.29316700	-1.80544600	1.61071100
C	0.24344800	-2.17689800	0.20247100
C	1.12782100	-1.26292600	-0.64835700
N	1.93785400	-0.44114900	0.03993100
O	1.10321500	-1.30125900	-1.87116900
H	0.07113400	-2.59446600	2.20003700
C	-1.17137600	-2.24899100	-0.40470000
C	-1.93189600	-0.96193700	-0.25404100
C	-1.75581300	0.08752400	-1.15548400
C	-2.42374500	1.29224700	-0.99004700

C	-3.28418300	1.47119200	0.08794200
C	-3.47655000	0.43750800	0.99507300
C	-2.80372600	-0.76241800	0.81630600
O	-3.96696000	2.63187300	0.29842100
H	0.69587600	-3.16630300	0.10752100
H	-1.07111700	-2.51209700	-1.45592400
H	-1.70947400	-3.05493400	0.09614500
H	-1.08636400	-0.04455700	-1.99343400
H	-2.28050000	2.09421000	-1.70366100
H	-4.15604300	0.58271200	1.82187900
H	-2.97242200	-1.56835400	1.51869700
H	-3.75598100	3.25721200	-0.40097900
H	-0.38131400	-1.07551800	1.80790400
C	2.84401200	0.43499100	-0.64278300
C	3.64422000	1.22849600	0.35102600
O	4.48622500	2.06946800	-0.27238000
O	3.56106900	1.13853500	1.54691900
H	1.94247400	-0.49368100	1.04814800
H	2.31054000	1.12598000	-1.29803200
H	3.53093700	-0.11820800	-1.28675500
H	4.97398500	2.54723900	0.41374900

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gasphase-5.xyz

N	0.11894400	2.05725300	-1.41607900
C	0.41960100	1.93052100	0.00476400
C	1.27448200	0.69771500	0.27805300
N	1.72020900	0.04165500	-0.79545900
O	1.54809900	0.35557500	1.43289600
H	0.03209100	3.02605300	-1.68461700
C	-0.81291200	1.92698100	0.93155800
C	-1.79817700	0.85027400	0.57361500
C	-2.89249000	1.12136900	-0.24252400
C	-3.78077200	0.12072400	-0.61977400
C	-3.58128400	-1.18025200	-0.17651500
C	-2.49736200	-1.47057000	0.64663000
C	-1.62034600	-0.46455500	1.01358500
O	-4.41222300	-2.20679400	-0.50508100
H	1.05106200	2.77349000	0.29165200
H	-0.46419700	1.80291700	1.95497200
H	-1.28853200	2.90501900	0.85349500
H	-3.06881600	2.13506700	-0.57809900
H	-4.63068500	0.35486300	-1.24816700
H	-2.36273800	-2.48398600	0.99512000
H	-0.78388900	-0.69522100	1.65815100
H	-5.12687100	-1.87929900	-1.05911000
H	-0.75385800	1.59241600	-1.63659600
C	2.46854300	-1.19737400	-0.70574100
C	3.91686500	-1.02084700	-0.24815500
O	4.07032900	-0.42828400	0.93542800
O	4.84639300	-1.41199900	-0.89891500
H	1.49250800	0.45290300	-1.68861000
H	2.48520200	-1.66534400	-1.68317400
H	1.96539900	-1.85982900	0.00121800
H	3.19175000	-0.19296300	1.31506900

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gasphase-6.xyz

N	0.28425300	-1.79911400	1.63379900
C	0.24192500	-2.18823500	0.22998900

C	1.13594400	-1.29069500	-0.62806900
N	1.93332800	-0.45048200	0.05235900
O	1.12637500	-1.35606100	-1.84982500
H	0.06071300	-2.58111800	2.23180200
C	-1.17024200	-2.25834500	-0.38447200
C	-1.92260000	-0.96435100	-0.25354100
C	-2.80454500	-0.75029500	0.80161900
C	-3.46883300	0.46103500	0.95766000
C	-3.25528800	1.48542000	0.04499100
C	-2.38214400	1.29014100	-1.02022300
C	-1.72612200	0.07921700	-1.16253400
O	-3.87566200	2.69547900	0.13696900
H	0.68808700	-3.18164700	0.15007500
H	-1.06573600	-2.53434800	-1.43200700
H	-1.71648400	-3.05472500	0.12287200
H	-2.99091500	-1.54730700	1.50958400
H	-4.15666800	0.60380300	1.78161100
H	-2.23393500	2.09224400	-1.72831800
H	-1.04774600	-0.06823300	-1.99077500
H	-4.45507800	2.70046700	0.90437700
H	-0.39249300	-1.06790100	1.81797500
C	2.83895300	0.42060200	-0.63772600
C	3.61587200	1.24532400	0.34906900
O	4.45773900	2.08108300	-0.28097000
O	3.51626400	1.18123000	1.54551800
H	1.92688000	-0.48178900	1.06133900
H	2.30624800	1.09036900	-1.31520600
H	3.54118700	-0.13859800	-1.25960300
H	4.92891700	2.58111900	0.40084000

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gasphase-7.xyz

N	0.24473500	-1.21194300	-0.42942700
C	0.27090800	0.24058100	-0.30619300
C	1.66619400	0.74320700	0.04100500
N	2.45830200	-0.16611100	0.66160200
O	1.99960400	1.89371800	-0.18244800
H	0.67440600	-1.50442000	-1.29766900
C	-0.69435700	0.69549800	0.79857400
C	-2.12430600	0.37111100	0.47377500
C	-2.83848900	1.14420500	-0.43876700
C	-4.14563100	0.83035300	-0.77943800
C	-4.76526900	-0.27619200	-0.20703600
C	-4.07147100	-1.05940000	0.70610000
C	-2.76492700	-0.73092300	1.03773800
O	-6.04660500	-0.63382300	-0.50069500
H	-0.00271500	0.76059000	-1.22853100
H	-0.40270900	0.20865600	1.73029100
H	-0.56487400	1.76978100	0.92516600
H	-2.36771500	2.00933900	-0.88679200
H	-4.68729600	1.44695900	-1.48566800
H	-4.56545900	-1.91116600	1.14971800
H	-2.23311100	-1.34065900	1.75614100
H	-6.41624800	-0.01149100	-1.13377700
H	-0.71084700	-1.54489700	-0.43384900
C	3.84900200	0.09530500	0.86587600
C	4.70004600	-0.38459300	-0.29092600
O	5.99658300	-0.09330900	-0.07914400
O	4.29893200	-0.95889400	-1.26575800

H	2.11600100	-1.11497200	0.64790600
H	4.20998500	-0.38132600	1.77692200
H	3.99459500	1.16872800	0.97163200
H	6.49270800	-0.41764500	-0.84434300

31

gasphase-8.xyz

N	0.05631900	-0.47022900	1.83620600
C	0.26332400	-1.02386400	0.50350800
C	1.74101400	-1.20246100	0.18688700
N	2.58892400	-0.51934100	0.99682100
O	2.11029200	-1.88566500	-0.75190300
H	0.17336000	-1.18224200	2.54476900
C	-0.30879100	-0.06838700	-0.55744000
C	-1.79261800	0.11358400	-0.41804200
C	-2.67452400	-0.87228900	-0.85506700
C	-4.04529300	-0.73348300	-0.69625200
C	-4.56125300	0.40693500	-0.08866000
C	-3.69981900	1.40269000	0.35270800
C	-2.33106200	1.24940400	0.18471400
O	-5.89768500	0.60069100	0.09403100
H	-0.19903100	-2.00508100	0.36177400
H	0.20196400	0.89111500	-0.46508200
H	-0.06160100	-0.48213700	-1.53376200
H	-2.28444200	-1.76062000	-1.33423200
H	-4.71557600	-1.50719500	-1.04920400
H	-4.11246900	2.28746700	0.81452100
H	-1.66582400	2.03342200	0.52139600
H	-6.38187000	-0.14885000	-0.26433300
H	-0.88574200	-0.11023600	1.92018500
C	3.95403300	-0.33961400	0.60864500
C	4.12685400	0.78843200	-0.38849500
O	5.40841700	0.87318700	-0.79046200
O	3.26040700	1.52577200	-0.76995800
H	2.14757000	0.13173600	1.62849200
H	4.32140400	-1.25420800	0.14782500
H	4.57749700	-0.12862800	1.47647800
H	5.46306200	1.60411700	-1.42264200

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gasphase-9.xyz

N	0.05042700	-0.48899800	1.82278100
C	0.26388200	-1.03709000	0.48862600
C	1.74315900	-1.20861600	0.17563200
N	2.58611100	-0.52796700	0.99317700
O	2.11785900	-1.88389700	-0.76659400
H	0.16487300	-1.20407000	2.52870000
C	-0.30792700	-0.07908700	-0.57014000
C	-1.79127200	0.10506100	-0.42897600
C	-2.32649900	1.25260900	0.14635900
C	-3.69884500	1.40550200	0.31113700
C	-4.56021400	0.39895000	-0.10416800
C	-4.04466400	-0.75637900	-0.68416500
C	-2.67645900	-0.89360800	-0.83993400
O	-5.91387900	0.48639900	0.02506200
H	-0.19461400	-2.01931700	0.34217700
H	0.20413200	0.87965100	-0.47664900
H	-0.06214100	-0.49151700	-1.54745200
H	-1.66288300	2.04565700	0.46421800
H	-4.09653500	2.30920900	0.75553600

H	-4.72675200	-1.52751800	-1.01059900
H	-2.28453400	-1.79227100	-1.29801300
H	-6.14375900	1.33215700	0.42076400
H	-0.89292800	-0.13145500	1.90291700
C	3.95123500	-0.33901700	0.60954700
C	4.12187100	0.80146600	-0.37367500
O	5.40369100	0.89554800	-0.77251600
O	3.25347500	1.54050300	-0.74765000
H	2.13993600	0.11798600	1.62672900
H	4.32210300	-1.24689900	0.13838200
H	4.57291000	-0.13647300	1.48070100
H	5.45677800	1.63389300	-1.39614900

31

gasphase-10.xyz

N	0.24319600	-1.19764100	-0.44282200
C	0.27157100	0.25469100	-0.31654200
C	1.66668800	0.75454100	0.03534100
N	2.45617100	-0.15805600	0.65486700
O	2.00195000	1.90528900	-0.18356800
H	0.67388900	-1.48892300	-1.31097300
C	-0.69527700	0.70796500	0.78748900
C	-2.12417400	0.37886900	0.46308300
C	-2.76705600	-0.70810600	1.04555700
C	-4.07676600	-1.03592900	0.71275000
C	-4.76496600	-0.26863000	-0.21750800
C	-4.13981700	0.82452700	-0.81020400
C	-2.83553600	1.13664400	-0.46924800
O	-6.04972400	-0.53241200	-0.58576100
H	0.00075600	0.77686400	-1.23839900
H	-0.40237100	0.22299500	1.71981200
H	-0.56901500	1.78281300	0.91299100
H	-2.24101600	-1.30706500	1.77700200
H	-4.56206600	-1.88289900	1.18110600
H	-4.68958000	1.41707600	-1.52645700
H	-2.35865100	1.99115300	-0.93114300
H	-6.37156500	-1.29823000	-0.10130400
H	-0.71342000	-1.52759700	-0.45036600
C	3.84674300	0.09996100	0.86436100
C	4.70269100	-0.40084300	-0.27965700
O	5.99955700	-0.11501500	-0.06268800
O	4.30474100	-0.98586000	-1.24946200
H	2.11237600	-1.10631400	0.63743300
H	4.20058400	-0.36415800	1.78472300
H	3.99569400	1.17434200	0.95510600
H	6.49890200	-0.45249000	-0.82006700

31

gasphase-11.xyz

N	-0.21120800	-0.70801300	1.17457700
C	-0.18058400	0.60673500	0.54828900
C	-1.57861200	1.10400300	0.20426400
N	-2.53620700	0.15777600	0.16405300
O	-1.78850200	2.27994300	-0.05153600
H	-0.49587800	-0.64205200	2.14270300
C	0.63074200	0.54907600	-0.75512500
C	2.07554100	0.21803000	-0.51421800
C	2.95568100	1.18727100	-0.03834500
C	4.28283500	0.88529500	0.22737600
C	4.75522200	-0.40702800	0.02037300

C	3.89474800	-1.38783700	-0.45507000
C	2.57018900	-1.06915700	-0.71780900
O	6.04784600	-0.76356700	0.26155000
H	0.25917300	1.38304700	1.18182500
H	0.17910700	-0.20203800	-1.40534100
H	0.53532900	1.51832900	-1.24247200
H	2.59988100	2.19659900	0.12133600
H	4.95415300	1.65354700	0.59004900
H	4.27471000	-2.38529300	-0.61947600
H	1.90759100	-1.83614500	-1.09659200
H	6.53844200	0.00182500	0.57491200
H	0.71070900	-1.12474700	1.15834300
C	-3.88198700	0.48998600	-0.20300400
C	-4.76777000	-0.71624500	-0.06922300
O	-6.03630300	-0.41989600	-0.39579300
O	-4.41005400	-1.81064400	0.27748000
H	-2.29006400	-0.79782800	0.37698800
H	-3.94457100	0.85693100	-1.22997400
H	-4.27525000	1.29127500	0.42467800
H	-6.55539400	-1.23078400	-0.29604900

31

gasphase-12.xyz

N	-0.20456300	-0.68140500	1.18815200
C	-0.18139800	0.62670700	0.54740100
C	-1.58225700	1.11217400	0.19844100
N	-2.53417200	0.15961400	0.16824200
O	-1.79971200	2.28398100	-0.06907500
H	-0.49022100	-0.60596400	2.15532200
C	0.62911800	0.55794800	-0.75596900
C	2.07339200	0.22639100	-0.51323600
C	2.56879000	-1.05528800	-0.72780100
C	3.89718700	-1.36977200	-0.46317900
C	4.75390600	-0.39183400	0.02394400
C	4.27798700	0.89755000	0.24310300
C	2.95297200	1.19401100	-0.02383300
O	6.06606200	-0.63183800	0.30071800
H	0.25468400	1.41206100	1.17211700
H	0.17617100	-0.19753400	-1.40021000
H	0.53483300	1.52358600	-1.25080400
H	1.91034100	-1.82168900	-1.11459700
H	4.26549400	-2.37214900	-0.64156700
H	4.95757900	1.65029500	0.61449500
H	2.59232100	2.20036000	0.14401600
H	6.27434500	-1.54828800	0.09698900
H	0.72067100	-1.09097300	1.17741000
C	-3.88177200	0.47971000	-0.20284800
C	-4.75723900	-0.73410100	-0.07008800
O	-6.02770600	-0.44912800	-0.39905100
O	-4.39068000	-1.82524400	0.27784200
H	-2.28203400	-0.79251100	0.38940400
H	-3.94430700	0.84483800	-1.23044500
H	-4.28428200	1.27827600	0.42249300
H	-6.53988800	-1.26441300	-0.29952900

31

gasphase-13.xyz

N	-0.02141300	-0.92577200	1.62987900
C	-0.26542900	0.31053100	0.89853600
C	-1.75064600	0.56033600	0.71002100

N	-2.55281200	-0.49493700	0.89228900
O	-2.16572900	1.66691200	0.35796600
H	-0.11855300	-0.78304800	2.62634300
C	0.37470900	0.23708500	-0.49824400
C	1.86969600	0.11490800	-0.43065000
C	2.50684100	-1.10018200	-0.65713900
C	3.88845600	-1.22009800	-0.55693500
C	4.65494000	-0.11074500	-0.22538700
C	4.03531800	1.11511600	0.00218100
C	2.65964000	1.21787000	-0.10053300
O	6.01027900	-0.15710100	-0.11300100
H	0.12497500	1.20004400	1.40117600
H	-0.04702700	-0.62103100	-1.02428300
H	0.08474900	1.13594600	-1.04029700
H	1.91914600	-1.96740000	-0.92778900
H	4.36698800	-2.17303300	-0.74354100
H	4.64494500	1.97157800	0.24935100
H	2.18774500	2.17668800	0.06993900
H	6.32058800	-1.04556600	-0.31132400
H	0.92357400	-1.24724000	1.46283800
C	-3.99726700	-0.41256400	0.78340100
C	-4.50418600	-0.29760100	-0.65450600
O	-4.04093400	0.74905700	-1.33713000
O	-5.28104200	-1.08190500	-1.12546300
H	-2.09712300	-1.36146700	1.13678800
H	-4.34242700	0.46190400	1.33820200
H	-4.43151400	-1.30587800	1.21719400
H	-3.42695500	1.27798000	-0.77627800

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gasphase-14.xyz

N	-0.02657500	-1.11146100	1.51790300
C	-0.26377100	0.19740500	0.92379100
C	-1.74777500	0.47444800	0.76569500
N	-2.55555600	-0.59011900	0.82993500
O	-2.15690800	1.61580400	0.53994200
H	-0.12593200	-1.07711700	2.52372200
C	0.37530100	0.27139200	-0.47353300
C	1.87068800	0.14657900	-0.42024700
C	2.65843900	1.22024700	-0.01166300
C	4.03717800	1.10568200	0.07938100
C	4.65607000	-0.09954100	-0.23921900
C	3.88845900	-1.18129100	-0.65133200
C	2.51025700	-1.05017700	-0.73893700
O	6.00407000	-0.27313800	-0.17070900
H	0.13184500	1.02599800	1.51826700
H	-0.04536800	-0.52815100	-1.08563300
H	0.08316700	1.22123300	-0.91868000
H	2.18891200	2.16437700	0.23145100
H	4.63440500	1.95317400	0.39113000
H	4.38076500	-2.10809700	-0.90593500
H	1.92027900	-1.89324300	-1.07381700
H	6.42154900	0.54695900	0.10869500
H	0.91698600	-1.41870000	1.31924000
C	-3.99977100	-0.48846000	0.73451300
C	-4.50976800	-0.20902900	-0.67959600
O	-4.04106700	0.90467500	-1.24185100
O	-5.29397100	-0.92987500	-1.23255700
H	-2.10455800	-1.48085300	0.97678900

H	-4.33920400	0.31945600	1.38546600
H	-4.43793600	-1.42282300	1.06575300
H	-3.42205200	1.36315000	-0.62711000

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gasphase-15.xyz

N	-0.12376100	-1.09293700	1.10647400
C	-0.28007900	0.14375100	0.35220800
C	-1.71394400	0.32964200	-0.11154800
N	-2.48144800	-0.76641100	-0.10389800
O	-2.11607400	1.42858200	-0.50017300
H	-0.41666300	-0.97072100	2.06684300
C	0.61598700	0.12411900	-0.89725900
C	2.07567300	0.08196400	-0.54726300
C	2.73233000	1.22739400	-0.10332600
C	4.06949100	1.19264200	0.26137900
C	4.77814200	-0.00304500	0.18836700
C	4.14209200	-1.15582500	-0.25421100
C	2.80420300	-1.10423700	-0.61707300
O	6.09136100	-0.10025800	0.53102300
H	-0.03348100	1.03924300	0.92911300
H	0.35015100	-0.74929800	-1.49528200
H	0.38524500	1.01369200	-1.48160100
H	2.19324900	2.16400800	-0.04821200
H	4.56556900	2.09440100	0.59723500
H	4.70466800	-2.07555700	-0.31547400
H	2.31905700	-2.00395300	-0.97232100
H	6.41768300	0.76086900	0.80839000
H	0.84898700	-1.37148900	1.12221500
C	-3.81402400	-0.79618700	-0.67833500
C	-4.87020900	-0.08991600	0.17204000
O	-4.62706800	1.19486300	0.42779500
O	-5.85890700	-0.64883400	0.56039900
H	-2.05171000	-1.60513900	0.25696600
H	-4.11999800	-1.82954600	-0.79309100
H	-3.78856400	-0.31643300	-1.65878600
H	-3.77366600	1.46939900	0.01798700

31

gasphase-16.xyz

N	-0.11841700	-1.07108300	1.11863500
C	-0.28091700	0.15755100	0.35226800
C	-1.71541000	0.33136800	-0.11409100
N	-2.47697400	-0.76888000	-0.09614800
O	-2.12336700	1.42396900	-0.51394000
H	-0.41106700	-0.94026800	2.07796900
C	0.61554400	0.12922200	-0.89669800
C	2.07505500	0.08892400	-0.54594400
C	2.80783600	-1.08962200	-0.63372800
C	4.14949400	-1.13388500	-0.27137400
C	4.77825800	0.01595500	0.18765500
C	4.06176800	1.20621000	0.27978900
C	2.72734400	1.23359500	-0.08359700
O	6.08773000	0.04407200	0.55601100
H	-0.03894200	1.05961500	0.92066200
H	0.34985300	-0.74820600	-1.48892500
H	0.38521400	1.01485600	-1.48727900
H	2.32971200	-1.98823500	-1.00074700
H	4.70499700	-2.05948000	-0.35243300
H	4.56607600	2.09465700	0.62990000

H	2.18061500	2.16494900	-0.01512500
H	6.47633800	-0.82738300	0.43541100
H	0.85616100	-1.34319300	1.13635700
C	-3.80877100	-0.81150300	-0.67146400
C	-4.86974000	-0.10335900	0.17133600
O	-4.63427600	1.18508200	0.41517200
O	-5.85552700	-0.66440600	0.56408300
H	-2.04326800	-1.60146300	0.27394700
H	-4.10888100	-1.84758600	-0.77686000
H	-3.78505400	-0.34073100	-1.65630300
H	-3.78219100	1.46083200	0.00349800

31

gasphase-17.xyz

N	0.11718600	-1.39125700	-0.89705300
C	0.25781800	0.02982700	-0.59888400
C	1.72598100	0.41629300	-0.46515500
N	2.61042300	-0.49058900	-0.89668900
O	2.06393000	1.50755100	-0.00104400
H	-0.77433100	-1.56741600	-1.33859300
C	-0.53286300	0.51179400	0.62660500
C	-2.00828200	0.30406800	0.44855900
C	-2.66919000	-0.76895700	1.03536800
C	-4.02727500	-0.98209400	0.82957000
C	-4.74786000	-0.11272500	0.02093500
C	-4.10557400	0.96868100	-0.57449100
C	-2.75291000	1.16680100	-0.35767800
O	-6.07919700	-0.26222100	-0.22105300
H	-0.10085700	0.58109700	-1.47147400
H	-0.17780600	-0.03581800	1.50292400
H	-0.30190300	1.56257100	0.79083000
H	-2.12177100	-1.44604800	1.67767600
H	-4.52493400	-1.81908900	1.30265500
H	-4.67959700	1.64352400	-1.19205200
H	-2.26530000	2.01718100	-0.81671200
H	-6.40998500	-1.02796900	0.25758500
H	0.12633800	-1.93057200	-0.03919600
C	4.03220800	-0.21338300	-0.98922400
C	4.74870500	-0.21960600	0.36108600
O	4.28197800	0.65206300	1.25481800
O	5.67871000	-0.94257300	0.59102600
H	2.22275900	-1.34561900	-1.26605400
H	4.17440800	0.76717700	-1.44802500
H	4.49413600	-0.97109900	-1.61135000
H	3.52622800	1.15714900	0.87481800

31

gasphase-18.xyz

N	-0.10350600	1.47446600	-0.78425200
C	-0.28970100	0.19589500	-0.10822700
C	-1.73210700	0.01931600	0.34875500
N	-2.61233600	0.90364400	-0.13447400
O	-2.05888100	-0.90829300	1.09306400
H	0.69773300	1.43113800	-1.39821900
C	0.67230700	-0.06291600	1.06174600
C	2.10054400	-0.10089000	0.60292600
C	2.61600000	-1.24175800	-0.00731100
C	3.91856700	-1.27843000	-0.48319700
C	4.73540600	-0.15980700	-0.35383100
C	4.24170700	0.98723900	0.25497000

C	2.93691900	1.00689800	0.72431100
O	6.02209800	-0.13347700	-0.79762200
H	-0.13374800	-0.58958400	-0.85133500
H	0.53522200	0.72897200	1.80221000
H	0.38851500	-0.99992700	1.53681800
H	1.99315100	-2.12131800	-0.10615500
H	4.30319200	-2.17741200	-0.94792900
H	4.88843600	1.84582300	0.35903100
H	2.56681900	1.90091000	1.20875500
H	6.24747000	-0.98481400	-1.18404500
H	0.08881600	2.20425500	-0.10832300
C	-4.01322400	0.90327900	0.24308100
C	-4.82915700	-0.22534900	-0.38850300
O	-4.39759300	-1.45703800	-0.11802100
O	-5.80208400	-0.01583700	-1.05907600
H	-2.25093000	1.57219500	-0.79808900
H	-4.45669700	1.84359500	-0.06346300
H	-4.08344900	0.80859300	1.32816600
H	-3.59642900	-1.41899700	0.45393400

31

gasphase-19.xyz

N	0.12394800	-1.44916600	-0.82206800
C	0.25661100	-0.01516000	-0.59026400
C	1.72281400	0.38668700	-0.48212900
N	2.61184600	-0.53505500	-0.87035400
O	2.05500200	1.50260300	-0.07592900
H	-0.76975000	-1.65241000	-1.24727800
C	-0.53211200	0.51875200	0.61504800
C	-2.00835900	0.30984200	0.44549000
C	-2.75881900	1.17712300	-0.34451000
C	-4.11487700	0.97121400	-0.55338700
C	-4.74838300	-0.11962800	0.03291200
C	-4.01873100	-0.99498300	0.82766600
C	-2.66402300	-0.77453000	1.02537300
O	-6.07555800	-0.37490000	-0.13119000
H	-0.10954600	0.49332200	-1.48550400
H	-0.17819600	0.00555400	1.51243800
H	-0.29785200	1.57449100	0.73624500
H	-2.27932300	2.03485300	-0.79812500
H	-4.68270800	1.66153000	-1.16425700
H	-4.52371300	-1.83193300	1.28675100
H	-2.10846000	-1.45428800	1.65790600
H	-6.46933200	0.30733000	-0.68287200
H	0.14496100	-1.94907200	0.05910400
C	4.03122900	-0.25306400	-0.98398600
C	4.75442200	-0.18354600	0.36103600
O	4.28480500	0.72915100	1.21116900
O	5.69207500	-0.88557100	0.62252100
H	2.22857600	-1.40939400	-1.19661300
H	4.16435300	0.70317200	-1.49405000
H	4.49580800	-1.03899800	-1.56795200
H	3.52297000	1.20782400	0.80977200

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gasphase-20.xyz

N	-0.09740200	1.44802300	-0.81053700
C	-0.29038500	0.17915000	-0.11800700
C	-1.73272000	0.01729100	0.34439500
N	-2.60786500	0.90351500	-0.14465200

O	-2.06383400	-0.90009700	1.09927700
H	0.69716500	1.38857300	-1.43171300
C	0.67133400	-0.06874000	1.05446900
C	2.10009500	-0.10783000	0.59750300
C	2.94723200	0.98246300	0.75789700
C	4.25651800	0.95592900	0.29157700
C	4.73736900	-0.17723200	-0.35151200
C	3.90579200	-1.28017700	-0.52091600
C	2.60533800	-1.23719700	-0.04918300
O	6.00812200	-0.27070800	-0.83057800
H	-0.14010100	-0.61679500	-0.85093700
H	0.53279500	0.72882300	1.78857100
H	0.38832000	-1.00219500	1.53720900
H	2.58839700	1.86661000	1.26810100
H	4.90283400	1.81274300	0.43364900
H	4.29499700	-2.15882500	-1.01362100
H	1.96993600	-2.10400900	-0.17740400
H	6.48544700	0.54213700	-0.64003700
H	0.10974600	2.18312300	-0.14483000
C	-4.00705000	0.91841200	0.23871600
C	-4.83515700	-0.20971400	-0.37771700
O	-4.41248100	-1.44211800	-0.09706800
O	-5.80965200	0.00132900	-1.04556000
H	-2.24361300	1.56247400	-0.81623500
H	-4.44417200	1.85918200	-0.07548600
H	-4.07338900	0.83526200	1.32500300
H	-3.60836800	-1.40526600	0.47076000

31

gasphase-4b.xyz

N	2.19532300	0.11179500	1.55648400
C	2.31822000	0.45563000	0.14231200
C	1.33292700	1.55828600	-0.25476800
N	0.71551300	2.17483500	0.77404100
O	1.16182400	1.88001600	-1.42040600
H	3.08010600	-0.20132300	1.92821000
C	2.20124500	-0.73864800	-0.82406000
C	0.97829500	-1.57267000	-0.55933900
C	1.07670600	-2.80109300	0.09318100
C	-0.04690900	-3.55508400	0.40027800
C	-1.30484000	-3.07502000	0.05999000
C	-1.42556300	-1.85113500	-0.58839100
C	-0.29389400	-1.11266300	-0.89692200
O	-2.38447300	-3.84193900	0.38613100
H	3.30031200	0.91016500	-0.00456000
H	2.19371600	-0.34617100	-1.83956900
H	3.09272800	-1.35623700	-0.70823000
H	2.05418700	-3.18132000	0.36053900
H	0.03617900	-4.50948100	0.89898400
H	-2.40443000	-1.46451900	-0.84165800
H	-0.40621700	-0.16146600	-1.39485700
H	-3.18641600	-3.39593600	0.09843500
H	1.53191900	-0.64594100	1.67252700
C	-0.23745300	3.21212500	0.53525100
C	-1.60413700	2.69437100	0.13310300
O	-1.94829800	1.54616300	0.09556900
O	-2.41501000	3.72525200	-0.17485400
H	0.88413600	1.79641700	1.69214400
H	0.11281400	3.85766700	-0.26903300

H	-0.35727400	3.82594400	1.42659500
H	-3.27147200	3.35101100	-0.42546800

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gasphase-4c.xyz

N	1.85578500	-0.17522200	-1.42190100
C	1.78310600	-0.41562600	0.01481600
C	0.52919000	-1.20762300	0.38821100
N	-0.15861700	-1.71625600	-0.65849500
O	0.19626500	-1.36974000	1.55139700
H	2.81325400	-0.04927000	-1.71636700
C	1.89911800	0.84356000	0.89433500
C	0.86596900	1.88151000	0.55807400
C	1.15484800	2.92694100	-0.31881200
C	0.19743700	3.86565200	-0.67515900
C	-1.08355500	3.76986800	-0.14774700
C	-1.39207900	2.73861100	0.73301000
C	-0.42543700	1.80574500	1.07909000
O	-1.99304500	4.71397600	-0.52120400
H	2.60648300	-1.08393600	0.27584900
H	1.80561700	0.53457800	1.93360700
H	2.89769200	1.25949900	0.75412700
H	2.15545700	3.01914400	-0.72091300
H	0.43016400	4.67758000	-1.34824000
H	-2.38827200	2.66826600	1.15192300
H	-0.67205800	1.00507700	1.76158800
H	-2.82934700	4.54359600	-0.07812000
H	1.34588500	0.66624400	-1.66408300
C	-1.21082000	-2.65932600	-0.44002800
C	-0.69972900	-4.07300000	-0.24971300
O	0.43936400	-4.43016500	-0.36216500
O	-1.71620000	-4.90393200	0.05112500
H	0.30006200	-1.64543500	-1.55383200
H	-1.90547600	-2.65858600	-1.27909700
H	-1.76571200	-2.38061500	0.45344400
H	-1.33935900	-5.78886500	0.15911100

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implicit-1.xyz

N	-0.16993700	-2.50617100	-1.37855000
C	-0.49698800	-2.35356100	0.03162300
C	-1.51050400	-1.24254100	0.24951700
N	-1.95014200	-0.60969200	-0.83314900
O	-1.89532800	-0.94496200	1.39562300
H	0.12042900	-3.45651300	-1.56357700
C	0.72101200	-2.14477400	0.95824100
C	1.53221500	-0.93564600	0.58588900
C	1.19622000	0.33288600	1.06001500
C	1.90880600	1.45981200	0.67449100
C	2.98253900	1.33283500	-0.20135400
C	3.34142000	0.07792600	-0.67980200
C	2.61809700	-1.03947300	-0.28448700
O	3.71700300	2.40490400	-0.61269700
H	-1.00717500	-3.26140900	0.35755100
H	0.36298100	-2.06344600	1.98298300
H	1.33454600	-3.04228000	0.88666300
H	0.36857700	0.44392300	1.74589700
H	1.63874300	2.43657300	1.05357400
H	4.18313700	-0.01439000	-1.35136100

H	2.91175700	-2.01318200	-0.65367500
H	3.37121200	3.20956800	-0.20806400
H	0.60548000	-1.90408600	-1.63132500
C	-3.04236500	0.34589200	-0.81570800
C	-2.68700700	1.68107300	-0.17752900
O	-2.20680300	1.62252200	1.05711100
O	-2.86222000	2.74075800	-0.73305600
H	-1.61210000	-0.95592500	-1.71995900
H	-3.88463400	-0.06843300	-0.25753300
H	-3.34919500	0.52773500	-1.83818000
H	-2.14812200	0.67015600	1.35256400

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implicit-2.xyz

N	0.14803200	2.18875200	-1.36687000
C	0.43342400	2.00936800	0.04920900
C	1.28747500	0.77683300	0.29055700
N	1.65112500	0.07675000	-0.77888100
O	1.63166500	0.45450900	1.44289200
H	-0.02152600	3.16594600	-1.56235100
C	-0.81455400	1.95766600	0.95851600
C	-1.76418800	0.85709400	0.57631200
C	-1.57597600	-0.44932200	1.02983700
C	-2.42138500	-1.47783800	0.63705700
C	-3.48041000	-1.21155500	-0.22569700
C	-3.69071700	0.08334600	-0.68511900
C	-2.83615400	1.10120900	-0.28267200
O	-4.34158100	-2.18234000	-0.64274300
H	1.04659800	2.84948000	0.37755700
H	-0.48474600	1.83774100	1.98901900
H	-1.31096600	2.92384400	0.87461100
H	-0.75894900	-0.66698900	1.70364500
H	-2.26577700	-2.48516600	1.00056900
H	-4.52070800	0.28420500	-1.34753500
H	-3.01327600	2.10771400	-0.63797500
H	-4.08845100	-3.02889600	-0.25568000
H	-0.69201100	1.68425700	-1.62720900
C	2.31809800	-1.20894000	-0.70853100
C	3.77075100	-1.13988400	-0.25977000
O	3.99279400	-0.50874300	0.88507100
O	4.67263600	-1.65713900	-0.87718600
H	1.39151300	0.45734900	-1.67758500
H	2.28494200	-1.66329800	-1.69101700
H	1.79109300	-1.85188500	-0.00038700
H	3.12941800	-0.17431300	1.26106700

31

implicit-3.xyz

N	-0.14612800	-2.50491900	-1.36404500
C	-0.48013700	-2.35170000	0.04438800
C	-1.50303100	-1.24805700	0.25607800
N	-1.94335900	-0.62057000	-0.82937200
O	-1.89475100	-0.95162500	1.40017600
H	0.14769000	-3.45457700	-1.54695200
C	0.73281900	-2.13241100	0.97523700
C	1.54041600	-0.92179500	0.59989800
C	2.63626300	-1.02731500	-0.25497900
C	3.35662400	0.09335700	-0.65232500
C	2.98230900	1.35026000	-0.19194300
C	1.89649800	1.47862000	0.66917700

C	1.18935600	0.35091500	1.05659600
O	3.64796200	2.48573900	-0.54618600
H	-0.98497300	-3.26249200	0.37040800
H	0.36978600	-2.04736100	1.99794700
H	1.35075500	-3.02742200	0.91109500
H	2.94202500	-2.00205000	-0.61131300
H	4.20775100	-0.00583200	-1.31302100
H	1.61841400	2.45884000	1.02981800
H	0.35239900	0.46175600	1.73112800
H	4.37236600	2.26408700	-1.14339900
H	0.62868000	-1.90070200	-1.61374900
C	-3.04343200	0.32611800	-0.81822100
C	-2.70229800	1.66528400	-0.18060500
O	-2.22358700	1.61244300	1.05495800
O	-2.88684500	2.72264000	-0.73748900
H	-1.59841700	-0.96519500	-1.71416300
H	-3.88466400	-0.09425500	-0.26299200
H	-3.34741500	0.50370300	-1.84228500
H	-2.15867300	0.66109100	1.35241500

31

implicit-4.xyz

N	0.30130900	-1.95018700	1.59391400
C	0.23695000	-2.28911400	0.17775000
C	1.15160700	-1.40365400	-0.66267300
N	1.86991300	-0.49989700	0.00858500
O	1.21184700	-1.52874600	-1.88761800
H	0.02589800	-2.74891500	2.14955700
C	-1.18680100	-2.28058800	-0.41875800
C	-1.87895500	-0.95713700	-0.25009400
C	-1.64834500	0.09863900	-1.13338200
C	-2.24992900	1.33647900	-0.95067000
C	-3.10045600	1.53923700	0.13212600
C	-3.34766900	0.50124400	1.02263700
C	-2.73841700	-0.73095300	0.82533300
O	-3.71951500	2.73286100	0.35880800
H	0.63592300	-3.29773700	0.06100100
H	-1.11590800	-2.54327400	-1.47286200
H	-1.75576600	-3.06142400	0.08543100
H	-0.98995500	-0.04931900	-1.97804100
H	-2.06626700	2.14459200	-1.64674200
H	-4.01565700	0.66373200	1.85662600
H	-2.94292100	-1.53560800	1.51914100
H	-3.46467000	3.36463900	-0.32399600
H	-0.35267900	-1.20547100	1.80833000
C	2.78399100	0.38724600	-0.65488100
C	3.35261100	1.37700300	0.32265200
O	4.18360000	2.22293000	-0.28339800
O	3.10131700	1.40638700	1.50363900
H	1.82007200	-0.50806500	1.01680200
H	2.28445800	0.93534300	-1.45419800
H	3.61458800	-0.15286400	-1.11383500
H	4.53834000	2.84266900	0.37395000

31

implicit-5.xyz

N	0.14264600	2.18187900	-1.38063600
C	0.43368000	2.01187000	0.03542800
C	1.29011800	0.78196200	0.28138900
N	1.64609300	0.07255900	-0.78453300

O	1.64253700	0.46986500	1.43402200
H	-0.02581300	3.15801200	-1.58219800
C	-0.81160900	1.96370100	0.94877900
C	-1.75805900	0.85590900	0.57993000
C	-2.83242200	1.08651300	-0.27721700
C	-3.68473400	0.05863200	-0.66467400
C	-3.46782400	-1.22979400	-0.19098900
C	-2.40430800	-1.48219300	0.67084800
C	-1.56322000	-0.44638600	1.04746900
O	-4.26910500	-2.27820000	-0.53225400
H	1.04633200	2.85504400	0.35663900
H	-0.47857300	1.85447700	1.97946700
H	-1.31195300	2.92717100	0.85713700
H	-3.01616000	2.08798900	-0.64313400
H	-4.51755700	0.25515400	-1.32706400
H	-2.24935100	-2.48548700	1.04185800
H	-0.74277300	-0.65185000	1.72100200
H	-4.96701800	-1.97383200	-1.12457100
H	-0.69973100	1.67746000	-1.63322100
C	2.31241400	-1.21310200	-0.70799100
C	3.76819500	-1.14168900	-0.26989900
O	3.99875300	-0.50119500	0.86799500
O	4.66522900	-1.66521300	-0.88911300
H	1.38041200	0.44567100	-1.68458200
H	2.27198500	-1.67562300	-1.68638500
H	1.78971300	-1.84953100	0.00919100
H	3.13842800	-0.16229700	1.24689800

31

implicit-6.xyz

N	0.29244500	-1.94599400	1.61577500
C	0.23594500	-2.29669300	0.20212600
C	1.15643000	-1.41949900	-0.64046700
N	1.86421000	-0.50413200	0.02623300
O	1.22865800	-1.55973000	-1.86309800
H	0.01693500	-2.74109400	2.17652100
C	-1.18474200	-2.28936900	-0.40222600
C	-1.87050300	-0.96001400	-0.25564900
C	-2.73104000	-0.71176900	0.81196500
C	-3.33244500	0.52971800	0.98655100
C	-3.07453200	1.55147600	0.08066400
C	-2.22222400	1.32499600	-0.99622400
C	-1.63007300	0.08143800	-1.15574000
O	-3.63468500	2.78932100	0.19646900
H	0.63303200	-3.30713700	0.09581000
H	-1.10958300	-2.56639100	-1.45239500
H	-1.75999400	-3.06067000	0.10943500
H	-2.94471400	-1.50309500	1.51820900
H	-4.00236500	0.70411500	1.81829100
H	-2.03453800	2.12348300	-1.70017400
H	-0.96969200	-0.08576200	-1.99523500
H	-4.19774500	2.81805600	0.97914300
H	-0.36500500	-1.20171200	1.82097900
C	2.77832700	0.38141700	-0.63926700
C	3.33624200	1.38196800	0.33354300
O	4.16641400	2.22732900	-0.27427100
O	3.07768100	1.41945400	1.51275300
H	1.80577700	-0.50098500	1.03401200
H	2.28145000	0.92050200	-1.44638600

H	3.61417200	-0.15874500	-1.08848200
H	4.51435700	2.85380900	0.38031500

31

implicit-7.xyz

N	0.17682800	-1.47585400	-0.40955400
C	0.27038100	-0.02212400	-0.35893600
C	1.68495200	0.44470000	-0.05678400
N	2.50516000	-0.46758800	0.47789200
O	2.02096200	1.61344200	-0.25143600
H	0.51580500	-1.81985700	-1.29950400
C	-0.64557700	0.53299600	0.74350300
C	-2.10270800	0.32349600	0.44344100
C	-2.74386900	1.09271300	-0.52778100
C	-4.08369300	0.89993100	-0.82957400
C	-4.81023700	-0.07744800	-0.15371800
C	-4.19114000	-0.85497200	0.81736400
C	-2.84811600	-0.64933500	1.10660200
O	-6.13006300	-0.30590800	-0.40641400
H	-0.00564800	0.45766400	-1.30220000
H	-0.38379400	0.04491900	1.68383300
H	-0.43440100	1.59669400	0.84589300
H	-2.19024000	1.85891700	-1.05459400
H	-4.57106400	1.50623700	-1.58209400
H	-4.76329800	-1.60795100	1.34046800
H	-2.37469800	-1.25230300	1.87021000
H	-6.43950500	0.30189000	-1.08849600
H	-0.79404700	-1.75669400	-0.34283600
C	3.84257400	-0.13710500	0.87064500
C	4.77917600	0.04235300	-0.30341300
O	5.95497000	0.52564300	0.10658200
O	4.52851800	-0.22032200	-1.45228100
H	2.15624500	-1.40772600	0.57497300
H	4.24120900	-0.93448600	1.49464900
H	3.85910400	0.78182400	1.45461700
H	6.54618600	0.60252500	-0.65906900

31

implicit-8.xyz

N	0.04858800	-0.40184100	1.82348900
C	0.25567000	-0.89124400	0.46721300
C	1.73236000	-1.02539900	0.13507300
N	2.57756400	-0.37014100	0.94177500
O	2.10576100	-1.68080000	-0.83815500
H	0.21593100	-1.14247900	2.49348000
C	-0.36586400	0.08236100	-0.54806300
C	-1.85845100	0.17622000	-0.40378700
C	-2.68328800	-0.84329300	-0.87837200
C	-4.06069600	-0.78787900	-0.72080800
C	-4.63855200	0.30247700	-0.07577900
C	-3.83525200	1.33008800	0.40351100
C	-2.45794400	1.25937700	0.23656100
O	-5.98543400	0.41000600	0.10575500
H	-0.17834800	-1.88072600	0.29569800
H	0.08621100	1.06480300	-0.40379000
H	-0.10467000	-0.26638700	-1.54631600
H	-2.24388200	-1.69390100	-1.38284900
H	-4.69025600	-1.58307500	-1.09811300
H	-4.29222800	2.17508900	0.89862000
H	-1.83943100	2.06531800	0.60873200

H	-6.42591600	-0.36259000	-0.26778700
H	-0.91680600	-0.11860800	1.93930200
C	3.98194200	-0.30997600	0.66882200
C	4.32199500	0.64248600	-0.45703600
O	5.61994800	0.56267900	-0.76373900
O	3.54744600	1.38577000	-1.00501400
H	2.17197900	0.19066300	1.67473600
H	4.36186300	-1.29431300	0.40163800
H	4.51176900	0.02125600	1.55948700
H	5.81483500	1.19807800	-1.47086300

31

implicit-9.xyz

N	0.04941000	-0.39818000	1.82129200
C	0.25782400	-0.88936600	0.46585900
C	1.73470600	-1.02418100	0.13496600
N	2.57950200	-0.36674200	0.94014400
O	2.10866700	-1.68197900	-0.83649100
H	0.21223100	-1.13882900	2.49235800
C	-0.36302400	0.08315300	-0.55074800
C	-1.85642800	0.17171400	-0.41242600
C	-2.46296200	1.25419600	0.21864200
C	-3.84347900	1.31878100	0.37606900
C	-4.63925200	0.28583600	-0.10356900
C	-4.05253000	-0.80580900	-0.73894900
C	-2.67550800	-0.85485000	-0.88673400
O	-5.99727800	0.29266900	0.01681700
H	-0.17601400	-1.87906100	0.29524700
H	0.08538500	1.06688400	-0.40389400
H	-0.09716600	-0.26376400	-1.54845800
H	-1.85135200	2.06529900	0.59092000
H	-4.30163200	2.16805200	0.86540200
H	-4.68078800	-1.60137100	-1.11384600
H	-2.22816900	-1.70552800	-1.38415100
H	-6.27968200	1.09872100	0.46544000
H	-0.91518900	-0.11106500	1.93435900
C	3.98429700	-0.30973600	0.66858700
C	4.32667900	0.63497400	-0.46310600
O	5.62410300	0.54868900	-0.77047200
O	3.55438800	1.37779900	-1.01489500
H	2.17408000	0.19407800	1.67315000
H	4.36382100	-1.29605200	0.40815500
H	4.51331700	0.02694100	1.55767900
H	5.82058000	1.17914300	-1.48157900

31

implicit-10.xyz

N	0.16967200	-1.37501700	-0.41308200
C	0.27145900	0.07753400	-0.36224500
C	1.68839700	0.52989700	-0.04740500
N	2.47580000	-0.38165100	0.53815900
O	2.05273100	1.68307100	-0.27881600
H	0.54872200	-1.72314300	-1.28522900
C	-0.65614200	0.63758600	0.72896600
C	-2.10564600	0.37491100	0.43384700
C	-2.80177900	-0.64467600	1.07732700
C	-4.13385800	-0.91094100	0.77869800
C	-4.78924700	-0.14802000	-0.17980300
C	-4.11176600	0.87809600	-0.83375000
C	-2.78429800	1.12943500	-0.52511600

O	-6.09385800	-0.35876200	-0.51447000
H	0.01042500	0.55944100	-1.30872300
H	-0.38117500	0.18152300	1.68122500
H	-0.47469600	1.70927900	0.80226100
H	-2.30073100	-1.24025700	1.82884800
H	-4.66363900	-1.70451100	1.28896700
H	-4.63236400	1.46948400	-1.57360500
H	-2.26629500	1.93020600	-1.03658800
H	-6.44614800	-1.09397200	0.00133600
H	-0.80491600	-1.64958600	-0.39127100
C	3.83318000	-0.09350800	0.89117200
C	4.76705600	-0.09734000	-0.29941300
O	5.99364400	0.28495700	0.06669400
O	4.46968500	-0.40847300	-1.42534800
H	2.10703400	-1.31496500	0.63326600
H	4.19003300	-0.83929600	1.59836200
H	3.90692900	0.88145200	1.36988400
H	6.57630200	0.25480500	-0.70869700

31

implicit-11.xyz

N	-0.22011400	-0.69268400	1.17479700
C	-0.18419900	0.61623000	0.53613400
C	-1.57930400	1.11011400	0.18549300
N	-2.53623100	0.17900600	0.15303100
O	-1.78333700	2.29548100	-0.08440700
H	-0.51327000	-0.60391400	2.14002500
C	0.63414500	0.55069300	-0.76372500
C	2.07711400	0.21497200	-0.51347700
C	2.95466800	1.17666700	-0.01324900
C	4.28226900	0.87238700	0.25188100
C	4.75509800	-0.41629000	0.01769400
C	3.89756500	-1.38986400	-0.47999400
C	2.57154300	-1.06820700	-0.74058600
O	6.04974600	-0.77085900	0.25581000
H	0.25244000	1.39219300	1.17168000
H	0.18507400	-0.20068100	-1.41523200
H	0.55251500	1.51839400	-1.25709500
H	2.59738500	2.18180900	0.16879500
H	4.95479400	1.62917900	0.63419700
H	4.27362500	-2.38645500	-0.66278400
H	1.91132000	-1.83028800	-1.13298900
H	6.53825600	-0.00973400	0.59099800
H	0.71108800	-1.09054700	1.19021300
C	-3.89148800	0.48990300	-0.20866400
C	-4.76284900	-0.72533600	-0.05791900
O	-6.02549900	-0.44959100	-0.37825700
O	-4.37877400	-1.81217000	0.30261500
H	-2.28384900	-0.77024900	0.38794500
H	-3.96382700	0.83626800	-1.24117300
H	-4.29506200	1.28402900	0.42054900
H	-6.56133000	-1.25206300	-0.27353600

31

implicit-12.xyz

N	-0.21876400	-0.69418400	1.17633500
C	-0.18459100	0.61449700	0.53734300
C	-1.58018400	1.10763800	0.18826500
N	-2.53680800	0.17631700	0.15587500
O	-1.78521300	2.29322100	-0.08028100

H	-0.51112900	-0.60549100	2.14181600
C	0.63281500	0.54901800	-0.76312400
C	2.07762200	0.22234200	-0.51205900
C	2.57935800	-1.05740200	-0.73232700
C	3.90915900	-1.36791800	-0.46838900
C	4.75972900	-0.38635000	0.02474500
C	4.27821800	0.90062000	0.25129700
C	2.95010500	1.19296700	-0.01582300
O	6.07316500	-0.62834500	0.29844800
H	0.25219900	1.39096300	1.17222000
H	0.18708100	-0.20685500	-1.41168600
H	0.54610600	1.51465900	-1.25969200
H	1.92554400	-1.82667600	-1.12132700
H	4.28639500	-2.36615900	-0.64696500
H	4.94947400	1.65871700	0.62928500
H	2.58495000	2.19635000	0.16059200
H	6.28141500	-1.54865100	0.09769000
H	0.71296400	-1.09091500	1.19099400
C	-3.89244300	0.48800000	-0.20378800
C	-4.76243000	-0.72919700	-0.06271000
O	-6.02500200	-0.45278700	-0.38296400
O	-4.37771400	-1.81810700	0.29084900
H	-2.28455900	-0.77315400	0.38998200
H	-3.96464500	0.84231200	-1.23357300
H	-4.29753800	1.27677500	0.43124500
H	-6.55965900	-1.25683400	-0.28441300

31

implicit-13.xyz

N	-0.02775400	-0.95704000	1.59203400
C	-0.26388500	0.27221000	0.85038500
C	-1.74459000	0.51964200	0.65148800
N	-2.55709700	-0.51567100	0.83814900
O	-2.15640600	1.63462200	0.28201600
H	-0.18303500	-0.80784300	2.58144000
C	0.39392500	0.19547800	-0.53867300
C	1.89031100	0.09764300	-0.44874800
C	2.54879100	-1.11228800	-0.64902100
C	3.93110400	-1.21065100	-0.53101300
C	4.67526100	-0.08328500	-0.20600400
C	4.03562900	1.13745000	-0.00414400
C	2.65764800	1.21831700	-0.12520600
O	6.03155200	-0.11532300	-0.07610100
H	0.11707600	1.16440100	1.35604900
H	-0.00597800	-0.67476700	-1.06136700
H	0.10540200	1.08651600	-1.09462300
H	1.97742700	-1.99415200	-0.90670200
H	4.43021100	-2.15686300	-0.69231000
H	4.62430800	2.00968000	0.24234000
H	2.16909100	2.17109800	0.03190900
H	6.35194300	-1.01117400	-0.23559500
H	0.93906500	-1.23915400	1.48781600
C	-4.00413400	-0.41975100	0.80249000
C	-4.58197900	-0.21362600	-0.58987300
O	-4.09312300	0.81241600	-1.27389900
O	-5.45974900	-0.90942000	-1.04505600
H	-2.12359600	-1.38404200	1.11823100
H	-4.32846000	0.42269100	1.41673800
H	-4.41537200	-1.33442700	1.21109200

H	-3.40405400	1.28769900	-0.73023900
31			
implicit-14.xyz			
N	-0.02947300	-1.11683400	1.49469400
C	-0.26309300	0.17938900	0.87658500
C	-1.74335600	0.44747200	0.70269400
N	-2.55673500	-0.60109700	0.77911700
O	-2.15379700	1.59517900	0.45038700
H	-0.18880500	-1.06553600	2.49334600
C	0.39345700	0.23691000	-0.51415300
C	1.88982100	0.12818300	-0.43700400
C	2.66096100	1.21429300	-0.02425700
C	4.04069300	1.11735500	0.08446500
C	4.67462900	-0.08455100	-0.22029200
C	3.92484600	-1.17841400	-0.63552400
C	2.54447000	-1.06425200	-0.74020700
O	6.02601900	-0.23694600	-0.13116300
H	0.11977700	1.01741000	1.46641300
H	-0.00887200	-0.57798200	-1.11793600
H	0.10597000	1.17803100	-0.98087900
H	2.17779100	2.15304500	0.21323200
H	4.62874600	1.96875100	0.40115200
H	4.42512800	-2.10593200	-0.87505100
H	1.96786400	-1.91870500	-1.06896100
H	6.42709600	0.58798500	0.16725900
H	0.93774000	-1.38768700	1.36705600
C	-4.00366400	-0.50142600	0.74957100
C	-4.57759100	-0.14912100	-0.61474200
O	-4.08774900	0.94382300	-1.18489700
O	-5.45359800	-0.79313600	-1.14371400
H	-2.12419800	-1.49394800	0.96944200
H	-4.32998000	0.27153600	1.44843100
H	-4.41612800	-1.45405000	1.05801700
H	-3.39981100	1.35875300	-0.59222600
31			
implicit-15.xyz			
N	-0.11417200	-1.10186200	1.12527600
C	-0.27976600	0.13460300	0.37611400
C	-1.71459800	0.31378300	-0.07583600
N	-2.48722700	-0.76817000	-0.05928700
O	-2.12501800	1.42250100	-0.46409700
H	-0.43245700	-0.98140500	2.07890800
C	0.60645000	0.12359000	-0.88205300
C	2.06910300	0.08284100	-0.54124100
C	2.72328100	1.22399600	-0.07810800
C	4.06568000	1.19218500	0.27078500
C	4.77975400	0.00164800	0.16092600
C	4.14691400	-1.14678900	-0.29916000
C	2.80251200	-1.09768800	-0.64506100
O	6.09993600	-0.08738700	0.48757700
H	-0.03450800	1.02785500	0.95696100
H	0.33929300	-0.74683400	-1.48314800
H	0.37773800	1.01755100	-1.46069700
H	2.17761300	2.15446700	0.00867100
H	4.56337600	2.08563500	0.62422000
H	4.70944200	-2.06545900	-0.38580600
H	2.31799700	-1.99458000	-1.00767000
H	6.41917500	0.77199300	0.78754400

H	0.86765300	-1.34426400	1.17398300
C	-3.80728600	-0.82283200	-0.65895600
C	-4.87326000	-0.05414600	0.10772000
O	-4.59896500	1.21801100	0.36384200
O	-5.92772300	-0.54648700	0.43597200
H	-2.06505000	-1.61598400	0.29223100
H	-4.11068700	-1.86081600	-0.71655800
H	-3.76872500	-0.40564300	-1.66737300
H	-3.70218200	1.45446800	-0.00509800

31

implicit-16.xyz

N	-0.11211100	-1.10667300	1.12104300
C	-0.27862400	0.12895000	0.37063800
C	-1.71376400	0.30803700	-0.08034100
N	-2.48862700	-0.77208400	-0.05646700
O	-2.12280800	1.41579700	-0.47298600
H	-0.42581400	-0.98430900	2.07593000
C	0.60830600	0.11724100	-0.88688400
C	2.07052700	0.08818900	-0.54319900
C	2.81496300	-1.08328200	-0.64848400
C	4.16043100	-1.11813700	-0.29764300
C	4.77908600	0.03500900	0.16904800
C	4.05225300	1.21800900	0.27962400
C	2.71265200	1.23572500	-0.07388100
O	6.09369100	0.06521200	0.52723900
H	-0.03363400	1.02275500	0.95076800
H	0.34728400	-0.75784400	-1.48388100
H	0.37481700	1.00698000	-1.47015800
H	2.34216200	-1.98460700	-1.01544500
H	4.72837300	-2.03461500	-0.38775300
H	4.54465900	2.11084600	0.63806300
H	2.15588700	2.15958300	0.01346500
H	6.48191000	-0.81025800	0.41131400
H	0.86949300	-1.35083700	1.16561000
C	-3.81129900	-0.82625600	-0.65041600
C	-4.87207600	-0.05124500	0.11722000
O	-4.59367900	1.22152900	0.36572000
O	-5.92616900	-0.53946700	0.45274000
H	-2.06734100	-1.61903000	0.29819200
H	-4.11750900	-1.86373000	-0.70188800
H	-3.77597500	-0.41391500	-1.66092600
H	-3.69787000	1.45400000	-0.00822800

31

implicit-17.xyz

N	0.10648200	-1.40537500	-0.94514100
C	0.25864200	0.00631900	-0.62331900
C	1.72439000	0.38389600	-0.48664400
N	2.61436100	-0.54213300	-0.83162400
O	2.06391500	1.50882400	-0.07679400
H	-0.78533900	-1.56218900	-1.39415800
C	-0.52071100	0.46369400	0.62137500
C	-2.00059500	0.28198300	0.44742900
C	-2.66672000	-0.81483500	0.98637200
C	-4.03123500	-0.99931900	0.79214000
C	-4.75062700	-0.07586800	0.04311900
C	-4.10382800	1.02775900	-0.50599200
C	-2.74297500	1.19667400	-0.30122400
O	-6.09039600	-0.20083900	-0.17936200

H	-0.09720800	0.58220400	-1.48080000
H	-0.16829500	-0.11804000	1.47569800
H	-0.28634500	1.50941100	0.81178100
H	-2.11643400	-1.53689900	1.57472700
H	-4.53722900	-1.85410300	1.22131500
H	-4.67274900	1.74398400	-1.08175100
H	-2.24921100	2.06002300	-0.72833600
H	-6.41914600	-0.99303700	0.26207300
H	0.10818200	-1.96048000	-0.09683200
C	4.03610700	-0.27862500	-0.95279600
C	4.75086700	-0.10290600	0.37863600
O	4.24189200	0.81293900	1.19200100
O	5.74427700	-0.72413200	0.67746400
H	2.24156200	-1.41776700	-1.16975400
H	4.19158500	0.63624700	-1.52858700
H	4.49135100	-1.10931400	-1.47756100
H	3.44660500	1.24064700	0.76627400

31

implicit-18.xyz

N	-0.10010800	1.39576500	-0.88245100
C	-0.29353000	0.12677400	-0.19605300
C	-1.73498300	-0.04270500	0.25213200
N	-2.60090500	0.88103700	-0.15394500
O	-2.08160700	-1.01796300	0.94353900
H	0.71251200	1.34258500	-1.48126100
C	0.64841600	-0.10360400	0.99972500
C	2.08859600	-0.11389500	0.57662500
C	2.64635400	-1.24764900	-0.01244400
C	3.96531800	-1.26142000	-0.44529100
C	4.75288400	-0.12401400	-0.29246600
C	4.21682000	1.01706800	0.29281900
C	2.89518200	1.01346100	0.71928300
O	6.05518800	-0.08041300	-0.69521500
H	-0.12545700	-0.67222600	-0.92113800
H	0.47642900	0.69312400	1.72629300
H	0.38393800	-1.04786200	1.47210900
H	2.04330000	-2.13832600	-0.13283400
H	4.38774800	-2.15028100	-0.89551000
H	4.83676500	1.89433000	0.41183700
H	2.48744100	1.90447400	1.17784200
H	6.30313300	-0.92811600	-1.08291500
H	0.07922100	2.13463800	-0.21177900
C	-3.97780200	0.94553200	0.29711600
C	-4.87463500	-0.14610600	-0.26834500
O	-4.45333400	-1.39092600	-0.08967800
O	-5.92780400	0.08759900	-0.81459200
H	-2.23960300	1.60240500	-0.76130700
H	-4.38500800	1.90643500	0.00769700
H	-4.00788900	0.85837200	1.38500400
H	-3.58351900	-1.38772200	0.40089900

31

implicit-19.xyz

N	0.10399900	-1.43648400	-0.88852000
C	0.25731500	-0.01451800	-0.61616100
C	1.72381200	0.36556200	-0.49404300
N	2.61168900	-0.57143700	-0.81436400
O	2.06581900	1.50161700	-0.11878100
H	-0.79025000	-1.60881900	-1.32694700

C	-0.52108600	0.48773900	0.61200300
C	-2.00039800	0.29297000	0.44766200
C	-2.75265900	1.18711800	-0.31272400
C	-4.11349400	0.99821700	-0.51233100
C	-4.74643600	-0.10490700	0.05307200
C	-4.01583400	-1.00730600	0.81726700
C	-2.65533800	-0.80287000	1.00646500
O	-6.07982100	-0.34152200	-0.10863300
H	-0.09895500	0.53109400	-1.49306900
H	-0.16459000	-0.05932400	1.48729400
H	-0.29023000	1.54082700	0.76125600
H	-2.27021100	2.04919200	-0.75496800
H	-4.68676400	1.70318300	-1.10028100
H	-4.51640200	-1.85818700	1.25719900
H	-2.09538300	-1.50829400	1.60584600
H	-6.46593500	0.34669000	-0.66322900
H	0.11049000	-1.96229900	-0.02173900
C	4.03342400	-0.31374700	-0.94709100
C	4.75200200	-0.10061200	0.37674200
O	4.24693300	0.83959900	1.16447000
O	5.74500400	-0.71479200	0.69100700
H	2.23686000	-1.45636100	-1.12496500
H	4.18870400	0.58357600	-1.54989200
H	4.48602000	-1.16020600	-1.44845300
H	3.45138800	1.25605100	0.72887300

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implicit-20.xyz

N	-0.09603700	1.41067800	-0.87186400
C	-0.28953400	0.13837200	-0.19169500
C	-1.73170900	-0.03605300	0.25211200
N	-2.59851000	0.88805500	-0.15111700
O	-2.07843500	-1.01692300	0.93550100
H	0.71556500	1.35998100	-1.47228300
C	0.65146200	-0.09629600	1.00382300
C	2.09066600	-0.12027300	0.57807900
C	2.91063000	0.99498300	0.72319800
C	4.23259100	0.98176900	0.29179300
C	4.75147900	-0.16358800	-0.30007600
C	3.94860000	-1.29023500	-0.45486800
C	2.63316400	-1.25977700	-0.01808700
O	6.03974600	-0.23883700	-0.74137800
H	-0.11953200	-0.65714000	-0.92020400
H	0.48663900	0.70367100	1.72845800
H	0.38026700	-1.03736900	1.47887200
H	2.51690800	1.88986300	1.18637500
H	4.86053400	1.85430500	0.41585100
H	4.36304400	-2.17837000	-0.91050800
H	2.01708000	-2.14134800	-0.13989400
H	6.48662100	0.60078500	-0.58096800
H	0.08483200	2.14590500	-0.19760900
C	-3.97809200	0.94380700	0.29275000
C	-4.86756300	-0.14652800	-0.28677900
O	-4.44235300	-1.39122700	-0.11662300
O	-5.91865100	0.08778600	-0.83673200
H	-2.23714600	1.61408600	-0.75284500
H	-4.38736500	1.90547800	0.00886000
H	-4.01391100	0.84758300	1.37969700
H	-3.57574000	-1.38900400	0.37929500

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implicit-4b.xyz

N	2.31219500	0.12245600	1.52192700
C	2.31967000	0.47079200	0.10633900
C	1.29487800	1.55358500	-0.22058100
N	0.65672200	2.09672800	0.82295900
O	1.10339800	1.92506400	-1.37943500
H	3.21258100	-0.25530500	1.78517400
C	2.16690700	-0.72845800	-0.85046600
C	0.95375700	-1.56600400	-0.55436400
C	1.06803200	-2.76127000	0.15603600
C	-0.04536100	-3.52847500	0.47280600
C	-1.30746900	-3.09881900	0.07975600
C	-1.44607500	-1.90800100	-0.62625000
C	-0.32306000	-1.15402000	-0.93693800
O	-2.37702500	-3.87909600	0.40935600
H	3.28171200	0.93911200	-0.10990200
H	2.13233200	-0.34792700	-1.87013300
H	3.06342700	-1.34022300	-0.75233000
H	2.04755400	-3.10343900	0.46308800
H	0.05533200	-4.45573300	1.01895800
H	-2.43056100	-1.57307500	-0.92578200
H	-0.44684800	-0.22589800	-1.47531600
H	-3.18692700	-3.47423700	0.07683800
H	1.62735300	-0.60377600	1.70056200
C	-0.26651900	3.17895700	0.65209900
C	-1.59614400	2.74330100	0.07618600
O	-1.98268000	1.60702500	-0.02607100
O	-2.31425700	3.81003500	-0.29352200
H	0.89441500	1.75591300	1.74070100
H	0.14904400	3.94283300	-0.00312300
H	-0.46222200	3.63916800	1.61874300
H	-3.17439600	3.50781700	-0.62565400

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implicit-4c.xyz

N	2.04244000	-0.17114300	-1.40692500
C	1.93208900	-0.41982200	0.02499000
C	0.69805800	-1.24771400	0.36538400
N	-0.05704200	-1.63277300	-0.67214300
O	0.42246500	-1.53296100	1.53106000
H	3.00426300	0.03263100	-1.64393000
C	1.96971100	0.84987200	0.90199900
C	0.87880200	1.82556700	0.56050300
C	1.10550200	2.87004900	-0.33629500
C	0.09407200	3.75032800	-0.69776600
C	-1.17685600	3.59444600	-0.15724400
C	-1.42574600	2.56328700	0.74351800
C	-0.40399600	1.69101000	1.09351200
O	-2.14224100	4.48019700	-0.53547300
H	2.77766400	-1.04496600	0.31610900
H	1.89666800	0.54659100	1.94495000
H	2.94342500	1.31674000	0.75475700
H	2.09418800	3.00519000	-0.75452000
H	0.28179100	4.55841300	-1.39048400
H	-2.41472400	2.44980800	1.16833900
H	-0.60680000	0.89270200	1.79360200
H	-2.97074900	4.26589500	-0.09041500
H	1.49836900	0.64451100	-1.66589300

C	-1.20493200	-2.46912600	-0.49050000
C	-0.84796800	-3.91189800	-0.20586700
O	0.25924300	-4.38517200	-0.26145500
O	-1.94118200	-4.61350100	0.10603800
H	0.30773800	-1.45522800	-1.59488100
H	-1.81547300	-2.44756500	-1.39091800
H	-1.81501300	-2.10547900	0.33426600
H	-1.68777600	-5.53763800	0.25951100

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explicit-1_co.xyz

N	-1.90326166185707	-0.50593317431767	-0.69184316555478
O	-2.06901571308849	-0.65945043418752	1.55050718427898
H	-0.18529444055742	-3.51313430519551	-1.08749970327082
C	0.64115270126915	-1.82193095551797	1.32586308593884
C	1.45067606080887	-0.69580098678616	0.74749427639449
C	1.04397424103723	0.62926811109708	0.89892182472328
C	1.73151423772807	1.66791817879606	0.29128757204817
C	2.85791818062472	1.39770576657838	-0.47937674423815
C	3.29497918060323	0.08708327700560	-0.62584158545411
C	2.59126007441120	-0.94215456726837	-0.01668523766007
O	3.57215335546002	2.37439836929331	-1.10188174169757
H	-1.06903761825088	-3.03859023185202	0.89849280488763
H	0.27132215084286	-1.57582760410578	2.31821660359391
H	1.25497523773453	-2.71735974548434	1.42064000749601
H	0.17784854665635	0.86100656020513	1.50052134391412
H	1.38827680311231	2.68699204517954	0.41617322427152
H	4.18107349356182	-0.10909715398466	-1.21126789935943
H	2.94718420074332	-1.95871879336135	-0.12600589970872
H	3.15919369132932	3.22751821265009	-0.93726119797081
H	0.69631067281751	-2.13444896216518	-1.18117944335592
C	-2.89365998551030	0.54360856071167	-0.83878928102432
C	-2.41018989739493	1.90404694218345	-0.33336461457837
O	-2.12540688960969	1.95297884020245	0.96997735273226
O	-2.31406117659213	2.86308173663809	-1.04719445953182
H	-1.46898048692290	-0.93511815593764	-1.49765805132377
H	-3.79343907957089	0.26694616336504	-0.28613993363175
H	-3.13449303477804	0.64726798591477	-1.89023756642216
H	-2.23065121872035	1.05878912705127	1.37007843607600
O	-1.79918002709041	-2.87863381822280	3.26526688373648
H	-2.43098813600355	-2.98507070622915	3.97856888202823
H	-1.99952418991089	-2.02173557375748	2.85641689109618

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explicit-2_co.xyz

N	1.63883200	-0.00985200	-0.68512600
O	1.62846300	0.05981600	1.56729800
H	0.27495800	3.18814200	-1.13252700
C	-0.78634900	1.69056300	1.26035600
C	-1.74948900	0.67498600	0.71422800
C	-1.58225600	-0.68490200	0.97471200
C	-2.43924400	-1.63037900	0.43095600
C	-3.48861400	-1.22939500	-0.39003800
C	-3.67831000	0.12070200	-0.65528100
C	-2.81391000	1.05480600	-0.10329900
O	-4.36170600	-2.11059700	-0.95025200
H	1.10731900	2.59657900	0.85080000
H	-0.48384800	1.43745200	2.27311500
H	-1.25869600	2.67188000	1.29963100

H	-0.77485000	-1.00575300	1.61827900
H	-2.29936000	-2.68112500	0.65219400
H	-4.50594300	0.42220800	-1.28010200
H	-2.98412000	2.10609500	-0.29679900
H	-4.13868900	-3.00465900	-0.67480800
H	-0.69686800	1.87854900	-1.28608900
C	2.30542300	-1.29351500	-0.78915800
C	3.78925500	-1.26430900	-0.42022400
O	4.06019100	-0.81526000	0.80576700
O	4.64363800	-1.64582300	-1.17059700
H	1.38377400	0.52034000	-1.50730600
H	2.22620200	-1.64297300	-1.81195400
H	1.80379600	-2.00273200	-0.12793500
H	3.22613600	-0.56883800	1.26622300
O	1.68861200	2.30946000	3.28289800
H	2.42225300	2.36420100	3.89817400
H	1.74118300	1.42672200	2.88503800

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explicit-3_co.xyz

N	0.69476800	-1.41036700	-1.41062700
O	0.75595400	-2.53942800	0.53857900
H	3.00493500	1.02039800	-0.45290400
C	1.08169200	0.13150900	1.74000700
C	-0.19493900	0.85553900	1.41740300
C	-0.23914200	2.24591400	1.37509900
C	-1.40058100	2.92359200	1.02136900
C	-2.54558900	2.20694500	0.69820500
C	-2.52451700	0.81588500	0.73918500
C	-1.36241000	0.15633400	1.09809200
O	-3.71430500	2.80709500	0.34381400
H	2.76059100	-0.80213500	0.79986700
H	0.89968800	-0.72133100	2.38940300
H	1.76537500	0.79776500	2.26546200
H	0.64250800	2.81504800	1.64038600
H	-1.41596400	4.00601900	1.00457200
H	-3.42103100	0.26707500	0.49151100
H	-1.36843500	-0.92327100	1.13674900
H	-3.60481500	3.76234000	0.36149200
H	1.42267000	1.44366100	-0.39822300
C	0.04637700	-2.46476900	-2.16738800
C	-1.42701800	-2.66202000	-1.80716700
O	-1.66014400	-2.98198300	-0.53217200
O	-2.30644600	-2.56309800	-2.61613100
H	1.01070200	-0.56090700	-1.85851500
H	0.57214600	-3.40526000	-1.99128500
H	0.09780000	-2.21666800	-3.22097000
H	-0.81217500	-3.01239900	-0.03231100
O	2.76347500	-2.58541100	2.51650400
H	3.02018100	-3.42940200	2.89223800
H	2.00412900	-2.76971400	1.94126400

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explicit-4_co.xyz

N	-1.91618262113813	-0.51994794239616	-0.67373697709174
O	-2.07606856692113	-0.74352848036470	1.56314722304877
H	-0.21255153724723	-3.51924206667747	-1.16962809182458
C	0.62975725086779	-1.90738161587181	1.29327669092181
C	1.44206497817388	-0.76703560028485	0.74752408809105
C	1.04092560777079	0.55427461111852	0.94084866212186

C	1.73118970793705	1.60855041155828	0.36400847521467
C	2.85479688204267	1.35793547591862	-0.41731160691305
C	3.28627430561515	0.05078048853433	-0.60540237079945
C	2.57983972067618	-0.99407553515375	-0.02673449431507
O	3.57152869275491	2.35064115498283	-1.01095116894208
H	-1.08599105723406	-3.10407407371607	0.83419023779782
H	0.26440961454080	-1.69051764637241	2.29409235270690
H	1.24036456327266	-2.80764348975673	1.35841921454575
H	0.17715939572598	0.77060967577213	1.55152354558798
H	1.39236250237362	2.62462947720737	0.52117844009812
H	4.17025992029178	-0.13057571671269	-1.19874312210166
H	2.93152293540799	-2.00813364554340	-0.16831649757945
H	3.16309022010236	3.19997677921878	-0.81793638802651
H	0.67687156288876	-2.14333071958017	-1.22166350139961
C	-2.90328419812059	0.53706846403651	-0.78449329748247
C	-2.41330989691655	1.87926329944213	-0.23829724879497
O	-2.12424822424539	1.88633951137265	1.06504046673399
O	-2.31546688198037	2.85972022529387	-0.92215349207671
H	-1.48537930968431	-0.92470356797779	-1.49393268025171
H	-3.80230384168177	0.24634581636176	-0.23787008503646
H	-3.14706697893912	0.67456740828632	-1.83137708926117
H	-2.23174731792055	0.98051364413361	1.43732573244531
O	-1.80455003891395	-3.01386808226148	3.20992162608158
H	-2.44960084787253	-3.14921641159929	3.90628929305273
H	-2.00390392343736	-2.14501413761556	2.82660008488256

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explicit-5_co.xyz

N	1.70712900	0.05912300	-0.88592100
O	1.84195600	0.39254700	1.33456500
H	0.15347300	3.12871900	-1.60800100
C	-0.64888500	1.94606600	1.01456800
C	-1.61027100	0.83433400	0.70212700
C	-2.68558000	1.03158000	-0.15988000
C	-3.54364300	-0.00866500	-0.49829800
C	-3.33329900	-1.27392300	0.03400800
C	-2.27569700	-1.48629900	0.91306800
C	-1.42833300	-0.44229900	1.24187200
O	-4.13380200	-2.33695000	-0.25416400
H	1.19540500	2.80982800	0.33582800
H	-0.28474600	1.85659900	2.03526400
H	-1.15157700	2.90997000	0.92628400
H	-2.87717100	2.01986100	-0.55804400
H	-4.37940800	0.16809900	-1.16340000
H	-2.14139500	-2.46908400	1.34051800
H	-0.63090200	-0.60694500	1.95211200
H	-4.83714600	-2.05901100	-0.84820800
H	-0.72328900	1.74793800	-1.54092700
C	2.42566100	-1.20073400	-0.88105400
C	3.92963400	-1.06045200	-0.64476700
O	4.27112100	-0.44213300	0.48721200
O	4.74336900	-1.49624300	-1.41035900
H	1.39051100	0.48158100	-1.74751200
H	2.28462400	-1.68456600	-1.84049900
H	2.01180500	-1.83449200	-0.09482600
H	3.46525600	-0.17844100	0.98420000
O	0.59418000	0.58010600	3.83860400
H	1.15727700	0.39728000	4.59287500
H	1.17000700	0.54286900	3.06000600

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explicit-6_co.xyz

N	1.86125900	-0.33575800	-0.11815800
O	1.26750800	-0.98349400	-2.18941700
H	0.17630100	-2.99393600	1.52869500
C	-1.16794900	-2.00162600	-0.92372300
C	-1.83097700	-0.71370200	-0.52594000
C	-2.69671800	-0.65360300	0.56197600
C	-3.27300800	0.54575700	0.96597100
C	-2.98608000	1.71476400	0.27441400
C	-2.12997500	1.67581600	-0.82168700
C	-1.56294000	0.47473900	-1.21162100
O	-3.51742400	2.92265900	0.61513000
H	0.64401400	-3.10720700	-0.65936100
H	-1.10147100	-2.08819800	-2.00517900
H	-1.75369100	-2.84843600	-0.56531700
H	-2.94259300	-1.56180700	1.09671400
H	-3.94971700	0.56814900	1.81090200
H	-1.92718600	2.59070400	-1.35898300
H	-0.90158800	0.45002600	-2.06647100
H	-4.09519600	2.81484800	1.37621900
H	-0.41540400	-1.46970600	1.48237000
C	2.75125000	0.68363900	-0.59304800
C	3.37356300	1.40505600	0.56955500
O	4.18502600	2.38664000	0.14493300
O	3.18627100	1.15051700	1.72919000
H	1.79135300	-0.53340200	0.87050900
H	2.22402600	1.40570400	-1.21837700
H	3.54635700	0.26736300	-1.21498600
H	4.55858500	2.81141600	0.93048900
O	0.62064900	-3.48612900	-3.22980700
H	1.12449800	-3.73558100	-4.00629800
H	0.87350100	-2.56600500	-3.03632500

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explicit-7_co.xyz

N	2.65446100	-0.29246300	0.65794700
O	2.26461000	1.84396500	0.01962600
H	0.73989500	-1.43572600	-1.36104800
C	-0.48179900	0.70505100	0.86911400
C	-1.91861900	0.50750800	0.47899500
C	-2.52186200	1.37854500	-0.42760600
C	-3.83581800	1.18723800	-0.82656700
C	-4.56967500	0.11593100	-0.32537000
C	-3.98478600	-0.75986200	0.57899600
C	-2.66893700	-0.55726900	0.97252400
O	-5.86438600	-0.11716300	-0.68449700
H	0.22986500	0.83840700	-1.14327700
H	-0.25107400	0.12985600	1.76762900
H	-0.29097300	1.75647600	1.07495300
H	-1.95150700	2.21370600	-0.81300700
H	-4.29611700	1.87392600	-1.52631600
H	-4.56695000	-1.58259800	0.96702300
H	-2.22139400	-1.23626000	1.68687800
H	-6.14992500	0.56238200	-1.30203800
H	-0.57433400	-1.47630500	-0.39734100
C	4.04330800	-0.08191600	0.92720700
C	4.91429000	-0.38541900	-0.27450800
O	6.20525500	-0.12758100	0.00281900

O	4.53046700	-0.80933000	-1.32899500
H	2.27196700	-1.22404200	0.58622100
H	4.37508900	-0.70477000	1.75700000
H	4.20117000	0.95778300	1.20672900
H	6.71801300	-0.33724700	-0.79100400
O	0.16198100	3.42243600	-0.91750700
H	0.97611500	2.97826900	-0.61613900
H	0.42868600	4.30598300	-1.17732300

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explicit-9_co.xyz

N	2.58733400	-0.51501000	0.91622200
O	2.06793800	-1.71195600	-0.93192800
H	0.11258500	-1.24683900	2.44456300
C	-0.33696500	0.10447200	-0.55450400
C	-1.82550400	0.22979100	-0.40340400
C	-2.40306400	1.32195700	0.23329400
C	-3.78158500	1.41276100	0.39899600
C	-4.59960700	0.39782400	-0.07753700
C	-4.03757800	-0.70209300	-0.71983600
C	-2.66522000	-0.78185400	-0.87788800
O	-5.95722200	0.42539800	0.05017100
H	-0.23328100	-1.88819900	0.22387200
H	0.14968700	1.06436500	-0.37357600
H	-0.08814500	-0.21815800	-1.56292400
H	-1.77206700	2.12294700	0.59590900
H	-4.21627000	2.27349500	0.89163400
H	-4.68949300	-1.47880000	-1.09205000
H	-2.22503900	-1.63169100	-1.38345000
H	-6.21903700	1.23821000	0.49217500
H	-0.83243900	-0.03742600	1.90142200
C	3.96578000	-0.36933200	0.56131700
C	4.20865300	0.83628100	-0.32439100
O	5.50049500	0.89334400	-0.69652200
O	3.38451700	1.64473600	-0.64897000
H	2.16733200	0.05883400	1.63295700
H	4.29674000	-1.25517200	0.02325200
H	4.58249500	-0.27020000	1.45336900
H	5.60415700	1.67570200	-1.25706600
O	-0.19478000	-2.79451000	-2.16507900
H	0.67141200	-2.48964700	-1.83800300
H	-0.00741500	-3.34780200	-2.92531600

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explicit-11_co.xyz

N	-2.47605800	0.39505700	0.18795500
O	-1.61923600	2.47954500	0.43460000
H	-0.49686900	-0.91183400	1.95986600
C	0.71377400	0.82426000	-0.60968500
C	2.13743200	0.37879800	-0.43720800
C	3.05184300	1.17302400	0.25076900
C	4.35873600	0.75510100	0.45192900
C	4.77530600	-0.47953200	-0.03639000
C	3.87967800	-1.28591500	-0.72658900
C	2.57618700	-0.85260200	-0.92108700
O	6.04510700	-0.94362300	0.12818600
H	0.34555100	1.23816300	1.46011800
H	0.23845900	0.25537400	-1.41032800
H	0.67101200	1.87920700	-0.87656500
H	2.74015700	2.13718600	0.63044500

H	5.05758000	1.38908800	0.98297700
H	4.21662100	-2.23841900	-1.10799800
H	1.88660400	-1.48197200	-1.46802400
H	6.56507900	-0.29339800	0.60943200
H	0.68369900	-1.22977700	0.88019400
C	-3.82809300	0.82052200	-0.06205200
C	-4.75492700	-0.35631700	0.04370900
O	-6.03261700	0.01968500	-0.11311000
O	-4.41516100	-1.49551600	0.23125500
H	-2.26269800	-0.59278400	0.21907800
H	-3.94360200	1.27530400	-1.04778000
H	-4.12851400	1.58517300	0.65486100
H	-6.57628300	-0.77914400	-0.05602900
O	-3.25710600	3.44098900	-1.60779500
H	-2.67624300	3.25605300	-0.84949900
H	-2.91495800	4.24096000	-2.00992800

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explicit-16_co.xyz

N	-2.58267593611954	-0.76665204800685	-0.10880670166895
O	-2.27523164408106	1.40285253903587	-0.64199255862287
H	-0.45612354500958	-0.79522299702276	2.06420782334340
C	0.49402587364203	0.13135234443594	-0.97437499770482
C	1.95239209567374	0.15474538271084	-0.61712689702944
C	2.72830986415002	-0.99764921764170	-0.65973742101658
C	4.07007296251969	-0.97567427759709	-0.29343105601514
C	4.64931947813995	0.21516004398054	0.12322206340477
C	3.88605804549237	1.37905824342237	0.16883758203829
C	2.55239804455902	1.34494575282834	-0.19699989680708
O	5.95657222813935	0.30806405783982	0.49391196840942
H	-0.15988218465776	1.13514502375252	0.79975524255637
H	0.25291411356787	-0.78696395986297	-1.51356426095243
H	0.24882681262923	0.97858972957961	-1.61145686169816
H	2.28774086649286	-1.92728266434898	-0.99619505747592
H	4.66250775146772	-1.88070562833787	-0.33841467145197
H	4.35523826488526	2.29841607368357	0.48706039073662
H	1.95871809497131	2.24922563724217	-0.17026851999642
H	6.37758030897743	-0.55204328900051	0.40574330294544
H	0.74695997730600	-1.27414945687114	1.07850957192117
C	-3.92093926380238	-0.86287049961903	-0.66260934078007
C	-4.98676566679427	-0.14755692838190	0.16792993542693
O	-4.77603609343976	1.15516594983700	0.36209520901313
O	-5.95491563027459	-0.71309584908677	0.59365113490245
H	-2.12948546056856	-1.56678546744714	0.31051302833315
H	-4.19687482202743	-1.90913031902176	-0.72304411728108
H	-3.92080893378994	-0.43138656638963	-1.66525061749308
H	-3.94087151042004	1.43371393523020	-0.07494125487030
O	-0.20698408613641	3.31855979903594	-0.53615417151840
H	-0.46050133204184	4.23499771916853	-0.66056332514980
H	-1.02298554709814	2.79916222407918	-0.62795019632354

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explicit-17_co.xyz

N	2.69678500	-0.61430400	-0.73727600
O	2.39841900	1.56507500	-0.24068000
H	0.17304100	-0.88037300	-2.40863700
C	-0.19217600	0.26276700	0.68055600
C	-1.69171600	0.21907200	0.61696200
C	-2.39651800	-0.94179100	0.91264000
C	-3.78375700	-0.98486800	0.81914300

C	-4.48144800	0.14823900	0.42372800
C	-3.79015000	1.31996800	0.12632300
C	-2.41044100	1.35069900	0.22213300
O	-5.83880300	0.17621300	0.31309300
H	0.06471900	1.13624500	-1.25632800
H	0.18776200	-0.59968300	1.23168400
H	0.13768800	1.16593200	1.18935400
H	-1.86083900	-1.82516600	1.23530900
H	-4.31839900	-1.89499600	1.05977000
H	-4.34973800	2.19468900	-0.17091600
H	-1.87140600	2.26230400	-0.00029300
H	-6.19891000	-0.68020000	0.56146600
H	-0.78098800	-1.31375100	-1.16408400
C	4.14517600	-0.58278000	-0.65456300
C	4.68234400	-0.47802500	0.77315500
O	4.26217900	0.58423900	1.46209700
O	5.44579800	-1.28119100	1.23167800
H	2.20192700	-1.46616700	-0.96288500
H	4.51085600	0.27495600	-1.22182700
H	4.53851100	-1.49386400	-1.09016800
H	3.66055400	1.13209100	0.91108900
O	0.27778500	3.42532500	-0.20801300
H	1.11558100	2.93366900	-0.18712100
H	0.50872300	4.34794000	-0.08526500

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explicit-4b_co.xyz

N	0.52598900	2.10477100	0.56726000
O	0.69282500	2.02296700	-1.67779500
H	3.30341200	0.05397100	1.19297900
C	1.82548100	-0.66396200	-1.31304500
C	0.70460000	-1.51452300	-0.78480700
C	0.96173100	-2.72566400	-0.14308200
C	-0.05870500	-3.49227600	0.40187100
C	-1.37007400	-3.04321900	0.31680000
C	-1.64837400	-1.83723600	-0.31675800
C	-0.61970900	-1.08707300	-0.86438100
O	-2.34323100	-3.82168400	0.87121600
H	3.02493600	1.02645000	-0.79222100
H	1.60930000	-0.29997600	-2.31452200
H	2.73818700	-1.25643900	-1.37638800
H	1.98127300	-3.08305400	-0.07721300
H	0.14548300	-4.43365700	0.89037000
H	-2.66617400	-1.47297100	-0.37278900
H	-0.85609100	-0.15078400	-1.34725800
H	-3.19719700	-3.39913600	0.74104100
H	1.82191100	-0.63477300	1.23483300
C	-0.45152000	3.14833200	0.55211100
C	-1.86131500	2.65635500	0.29340300
O	-2.21358000	1.51413700	0.20210900
O	-2.69877500	3.70604200	0.18866100
H	0.88517500	1.70613900	1.42114700
H	-0.21230200	3.86956800	-0.22842600
H	-0.44854100	3.67548600	1.50470900
H	-3.58422000	3.35148000	0.02489800
O	2.96556800	1.70463100	-3.27061000
H	2.09204000	1.87735900	-2.87863700
H	3.06529400	2.34645500	-3.97568100

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explicit-4c_co.xyz

N	-0.17696600	-1.61125500	-0.49248400
O	-0.09338900	-1.41460600	1.75471900
H	3.03635400	-0.24492100	-1.05309300
C	1.62794000	0.90248300	1.29097600
C	0.63653600	1.87767000	0.72268600
C	1.03492900	2.88411500	-0.15690700
C	0.12147700	3.76054600	-0.72515500
C	-1.22619900	3.64127700	-0.41308100
C	-1.64547100	2.64974200	0.46785900
C	-0.72106800	1.77960700	1.02670900
O	-2.08958400	4.52390600	-0.99052000
H	2.45222800	-1.04157300	0.95639300
H	1.38877000	0.66217300	2.32360900
H	2.62642200	1.34005500	1.28332000
H	2.08599700	2.99802000	-0.38887700
H	0.43832700	4.54321200	-1.39856000
H	-2.69477400	2.56337700	0.72158600
H	-1.05487500	1.01298800	1.71179900
H	-2.98177200	4.34862400	-0.67749000
H	1.67699500	0.63838800	-1.27172500
C	-1.30795200	-2.48635900	-0.46579700
C	-0.92346000	-3.93332300	-0.23134100
O	0.19357600	-4.36179200	-0.15989000
O	-2.02693100	-4.69820100	-0.12587500
H	0.39450600	-1.50889600	-1.31857300
H	-1.85525700	-2.42506300	-1.40512700
H	-1.98226600	-2.18634000	0.33383000
H	-1.73153400	-5.60855200	0.01865000
O	2.08642900	-1.45940000	3.51080900
H	1.23301800	-1.49268600	3.04564800
H	2.14028800	-2.27953900	4.00464800

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explicit-1_cocarb.xyz

N	-1.76383000	-0.76808900	-0.95196300
O	-2.11778800	-1.10409700	1.25281600
H	0.17398400	-3.68615000	-1.36845000
C	0.67689100	-2.07922500	1.14741000
C	1.27248100	-0.75419600	0.76602200
C	0.70017000	0.42191000	1.24719000
C	1.06155400	1.66027900	0.74890000
C	2.02118800	1.75686900	-0.25950600
C	2.66806800	0.59928400	-0.68909700
C	2.29191900	-0.63659400	-0.17994100
O	2.35393600	2.93433900	-0.82583100
H	-0.93442200	-3.38424200	0.53807500
H	0.25902900	-2.03377400	2.15162000
H	1.42243100	-2.87496100	1.12362500
H	-0.06248100	0.36389100	2.00936600
H	0.58420600	2.55571000	1.11576700
H	3.44357900	0.68241000	-1.43655000
H	2.80414900	-1.52521600	-0.52900500
H	1.63551200	3.57936600	-0.66897800
H	0.85790800	-2.19832500	-1.37980000
C	-2.74373900	0.28897700	-1.09661600
C	-2.31811100	1.57551300	-0.39202200
O	-2.27819700	1.51594800	0.92762100

O	-2.05517700	2.58631000	-1.00037600
H	-1.26120100	-1.12413900	-1.75175300
H	-3.69851800	-0.03789700	-0.68049200
H	-2.86405900	0.50879900	-2.15095800
H	-2.38241700	0.57260900	1.22114900
O	0.04752000	4.43188900	-0.58629300
H	-0.21868300	5.14351900	-0.00143000
H	-0.73337600	3.86175800	-0.69648500

31

explicit-2_cocarb.xyz

N	1.77235300	0.16563500	-0.84966600
O	1.61950200	0.39611300	1.38973500
H	0.00764900	3.12616100	-1.62378400
C	-0.79415600	1.91163500	0.96638400
C	-1.74337400	0.81115400	0.58386900
C	-1.52624600	-0.50234100	0.99898800
C	-2.37347500	-1.52732400	0.60415400
C	-3.46118600	-1.25497900	-0.21955200
C	-3.69921900	0.04821900	-0.63796900
C	-2.84493100	1.06335000	-0.23407700
O	-4.32629000	-2.21806800	-0.63768400
H	1.03688800	2.83831000	0.34073300
H	-0.43192500	1.77011400	1.98275600
H	-1.30440100	2.87404400	0.92161400
H	-0.68685300	-0.72207900	1.64346300
H	-2.19466500	-2.53988500	0.94347600
H	-4.55538800	0.25096200	-1.26411900
H	-3.05088200	2.07848000	-0.54802400
H	-4.06597800	-3.06794200	-0.27024100
H	-0.75456000	1.67844900	-1.61237800
C	2.53188300	-1.06852700	-0.81370200
C	3.97010600	-0.90617900	-0.32621000
O	4.11506800	-0.35974200	0.87195500
O	4.90847900	-1.27995300	-0.98077300
H	1.51256200	0.59654200	-1.72523800
H	2.56657500	-1.48598100	-1.81319100
H	2.02952500	-1.77365600	-0.14811500
H	3.23034600	-0.13023900	1.25202600
O	7.36367800	-2.39174000	-2.10686300
H	7.98821600	-2.13290500	-1.42712900
H	6.51909500	-2.03975400	-1.80301400

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explicit-3_cocarb.xyz

N	-2.22605100	-0.27952500	-0.66365400
O	-2.18962400	-1.20099300	1.39754000
H	-0.45296700	-2.98651700	-2.13795900
C	0.52472400	-2.00756500	0.56193900
C	1.20511000	-0.69520600	0.28861500
C	2.19391800	-0.58088000	-0.68497300
C	2.76380900	0.64846500	-0.99789300
C	2.34926500	1.79363200	-0.32713200
C	1.36619100	1.69956600	0.65489100
C	0.81251800	0.46700600	0.95659100
O	2.86527100	3.02548900	-0.58281900
H	-1.18404400	-3.16117000	-0.04369300
H	0.25967500	-2.08885300	1.61460500
H	1.19110500	-2.83434100	0.31474000
H	2.54060100	-1.46623400	-1.20189800

H	3.53616600	0.71364300	-1.75355200
H	1.04618300	2.59272300	1.17104300
H	0.05646200	0.41146700	1.72536000
H	3.52113300	2.96470200	-1.28379800
H	0.25197100	-1.52052800	-1.93346900
C	-3.14909500	0.78066300	-0.31944800
C	-2.50202900	1.82241800	0.59052200
O	-2.26550200	1.41477300	1.83308000
O	-2.21432700	2.93143400	0.21456400
H	-1.78713100	-0.26434000	-1.57211000
H	-4.01723600	0.35405900	0.18389000
H	-3.46141200	1.27185100	-1.23325300
H	-2.41047800	0.43659500	1.88868900
O	-0.70530300	1.84665100	-2.11327600
H	-1.16006900	2.48737400	-1.54969500
H	0.15015400	1.73050900	-1.68705000

31

explicit-4_cocarb.xyz

N	1.75097900	0.34300800	0.40339500
O	1.52247900	-0.99489600	-1.40776600
H	0.08785400	-2.18038700	2.56165600
C	-0.77823600	-2.13180100	-0.08863200
C	-1.73325000	-0.97269300	-0.10332900
C	-1.64199800	0.01667900	-1.08148900
C	-2.48976300	1.11445100	-1.07035300
C	-3.44990500	1.24380000	-0.07228200
C	-3.56005800	0.26726600	0.90928800
C	-2.70677900	-0.82597700	0.88448200
O	-4.30987000	2.29841200	-0.01227600
H	1.17347600	-2.69068600	0.60218800
H	-0.54397400	-2.44885600	-1.10298400
H	-1.22826000	-2.97801900	0.43289500
H	-0.89683100	-0.07644000	-1.85904500
H	-2.40890000	1.87028300	-1.84156500
H	-4.31729400	0.37155400	1.67218700
H	-2.81226300	-1.59091400	1.64287000
H	-4.13869800	2.89331600	-0.74821800
H	-0.31037600	-0.67643500	2.09542300
C	2.67581200	1.20931000	-0.26606300
C	4.11107400	0.75425500	-0.10138800
O	4.93468300	1.48108500	-0.87007200
O	4.49233000	-0.12218200	0.63026200
H	1.77390200	0.35461400	1.41362900
H	2.60056900	2.22145300	0.13006400
H	2.44683200	1.24208100	-1.32813900
H	5.83593200	1.16506500	-0.71052100
O	2.80693600	-0.09783300	3.14630300
H	2.09765900	-0.73887700	2.97736200
H	3.52197300	-0.34766000	2.54892500

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explicit-5_cocarb.xyz

N	2.02243000	-0.22469600	-0.52965500
O	1.70277300	0.55759500	1.56085000
H	0.36546700	2.53332700	-2.11494700
C	-0.62233500	1.94030200	0.56811800
C	-1.56334700	0.78788400	0.36062300
C	-2.57191600	0.84689100	-0.59655300
C	-3.41407800	-0.23430100	-0.82925700

C	-3.25449800	-1.40225300	-0.09497300
C	-2.25660200	-1.47918200	0.87157600
C	-1.42454000	-0.39507400	1.09181500
O	-4.04560000	-2.49653800	-0.26947000
H	1.28751800	2.68226600	-0.06462300
H	-0.36193400	2.03706500	1.62046400
H	-1.09763000	2.86928200	0.25141000
H	-2.71690400	1.75794100	-1.16227800
H	-4.19780200	-0.16463500	-1.57293600
H	-2.15203800	-2.38951300	1.44336900
H	-0.65302600	-0.45924500	1.84616100
H	-4.69752700	-2.31687800	-0.95323500
H	-0.28891800	1.05397000	-1.87682500
C	2.80133500	-1.36270300	-0.08980800
C	4.20888900	-0.95105100	0.32810100
O	4.27698400	-0.20854700	1.42513500
O	5.19413000	-1.26241100	-0.29719400
H	1.98971500	-0.00292800	-1.51527900
H	2.86894500	-2.07010700	-0.90635100
H	2.29856200	-1.82421400	0.76017600
H	3.36417300	0.02620700	1.72172700
O	3.87028900	-0.86795300	-2.81427700
H	4.32410600	-0.47786200	-3.56337900
H	4.55866700	-1.07904500	-2.16515300

31

explicit-6_cocarb.xyz

N	1.820167	-0.574946	0.292938
O	1.191858	-1.186077	-1.786601
H	-0.253274	-2.973074	1.957012
C	-1.230832	-2.254604	-0.684424
C	-1.991250	-0.983494	-0.431757
C	-2.973368	-0.918117	0.552087
C	-3.648510	0.266115	0.825960
C	-3.344040	1.413914	0.106523
C	-2.369515	1.368811	-0.885172
C	-1.704107	0.183086	-1.146471
O	-3.968782	2.606126	0.322343
H	0.568413	-3.273711	-0.121799
H	-1.029490	-2.373978	-1.747242
H	-1.822521	-3.109156	-0.353297
H	-3.229891	-1.810354	1.108203
H	-4.414742	0.292607	1.590574
H	-2.150613	2.266745	-1.444239
H	-0.947319	0.152299	-1.917329
H	-4.626850	2.501145	1.015566
H	-0.660364	-1.408395	1.729267
C	2.783015	0.379942	-0.173153
C	3.391503	1.121938	0.983923
O	4.259619	2.035971	0.579146
O	3.119339	0.900220	2.146725
H	1.715373	-0.747394	1.281739
H	2.324046	1.099500	-0.852598
H	3.586880	-0.096198	-0.739175
H	4.633811	2.488070	1.374280
O	4.913973	2.807355	3.073350
H	4.232143	2.142424	3.261399
H	4.658935	3.609270	3.534832

31

explicit-7_cocarb.xyz

N	2.565392	-0.357156	0.481774
O	2.221054	1.469371	-0.815889
H	0.741332	-1.933766	-1.272875
C	-0.510613	0.593690	0.482546
C	-1.959977	0.269159	0.259934
C	-2.683183	0.903202	-0.747360
C	-4.010144	0.582173	-0.991420
C	-4.640790	-0.391285	-0.223203
C	-3.937977	-1.034635	0.787164
C	-2.611669	-0.700886	1.019514
O	-5.941689	-0.748601	-0.414030
H	0.109541	0.285533	-1.547030
H	-0.202657	0.262934	1.475447
H	-0.348492	1.669748	0.421027
H	-2.203477	1.663968	-1.348964
H	-4.557954	1.089960	-1.775273
H	-4.439969	-1.783969	1.381161
H	-2.072033	-1.202027	1.812114
H	-6.313019	-0.232952	-1.135783
H	-0.624830	-1.829577	-0.365843
C	3.919690	-0.025147	0.786306
C	4.918351	-0.530421	-0.231928
O	6.166533	-0.199686	0.126332
O	4.668299	-1.152699	-1.232026
H	2.179096	-1.265373	0.692362
H	4.204077	-0.421202	1.760355
H	4.024155	1.058592	0.826839
H	6.765373	-0.532694	-0.557897
O	2.250706	-1.201226	-2.805190
H	3.077391	-1.278872	-2.307080
H	2.187724	-0.262791	-3.003841

31

explicit-9_cocarb.xyz

N	2.52665600	-0.45911700	0.91195900
O	2.01973700	-1.92317300	-0.74858900
H	0.17280600	-1.07383600	2.56264300
C	-0.42334600	-0.13769900	-0.57765000
C	-1.90496600	0.02989700	-0.40174200
C	-2.44344900	1.19510800	0.13363600
C	-3.81288900	1.33369200	0.33216100
C	-4.66813200	0.29435100	-0.00825100
C	-4.14941100	-0.87920100	-0.54733600
C	-2.78414800	-1.00168200	-0.73739400
O	-6.01879300	0.36599400	0.15724400
H	-0.25114600	-2.01997200	0.43956200
H	0.07406300	0.83294700	-0.55264100
H	-0.19929700	-0.60020400	-1.53762800
H	-1.78488800	2.01306500	0.39375200
H	-4.21329400	2.25122000	0.74468200
H	-4.82699400	-1.67632000	-0.81555100
H	-2.38995600	-1.91512700	-1.16310400
H	-6.25182200	1.22553700	0.52001600
H	-0.93161000	-0.06357200	1.91458700
C	3.87980400	-0.28032300	0.48238700
C	4.02821100	0.81604500	-0.55303300
O	5.28459300	0.92625600	-0.96401900
O	3.11299400	1.50909400	-0.94255900

H	2.09190800	0.21567800	1.52265800
H	4.24025000	-1.20593800	0.03812200
H	4.52553000	-0.04220800	1.32658300
H	5.33402000	1.64626000	-1.63793100
O	4.72355500	2.88450700	-2.73190400
H	3.85585900	2.72245200	-2.32614600
H	4.89296300	3.82663900	-2.66574200

31

explicit-11_cocarb.xyz

N	-2.560571	-0.372696	-0.572588
O	-2.234604	1.223965	1.003193
H	-0.697685	-2.182575	0.895002
C	0.499004	0.615669	-0.437511
C	1.955013	0.282560	-0.281068
C	2.679187	0.756866	0.809959
C	4.012983	0.421494	0.988690
C	4.649694	-0.405143	0.068456
C	3.945959	-0.887800	-1.027219
C	2.612784	-0.541688	-1.192426
O	5.957370	-0.768099	0.189078
H	-0.098214	-0.025652	1.519964
H	0.186299	0.444764	-1.468578
H	0.321503	1.664883	-0.201681
H	2.194875	1.402865	1.530321
H	4.561337	0.804580	1.840114
H	4.452588	-1.523459	-1.738277
H	2.072255	-0.916672	-2.051373
H	6.328433	-0.370569	0.982158
H	0.658565	-1.909937	0.008101
C	-3.921456	-0.017262	-0.814473
C	-4.906933	-0.699432	0.109218
O	-6.161819	-0.334831	-0.187647
O	-4.642490	-1.473199	0.993080
H	-2.161910	-1.227764	-0.930818
H	-4.205178	-0.252479	-1.839517
H	-4.043309	1.056495	-0.675764
H	-6.752301	-0.785286	0.433713
O	-2.212906	-1.730028	2.530140
H	-3.041578	-1.747700	2.029754
H	-2.166871	-0.831556	2.868932

31

explicit-16_cocarb.xyz

N	-2.84586300	-0.45255600	-0.36830200
O	-2.24637400	1.64838900	-0.93609500
H	-1.02864600	-0.59009300	1.97661800
C	0.36962000	0.04985700	-0.97895700
C	1.78888700	-0.08360900	-0.50712500
C	2.39781200	-1.32829700	-0.38950800
C	3.69868500	-1.45303200	0.08523400
C	4.41164400	-0.31887200	0.45076300
C	3.82001800	0.93611400	0.33791100
C	2.52431700	1.04340400	-0.13524200
O	5.68860900	-0.36946100	0.91984700
H	-0.31266100	1.24284700	0.66565600
H	0.05801600	-0.86235300	-1.48999300
H	0.27438800	0.87866000	-1.67931100
H	1.85303600	-2.21682000	-0.67991200
H	4.15778300	-2.43027000	0.16440400

H	4.38912300	1.81021600	0.61797200
H	2.07468300	2.02358200	-0.22544700
H	5.98867700	-1.28297000	0.93927100
H	0.32002700	-1.15876800	1.25473600
C	-4.15846600	-0.35219000	-0.97139700
C	-5.09407200	0.50790600	-0.12823800
O	-4.78993600	1.79769700	-0.08453500
O	-6.03776400	0.05125000	0.47205300
H	-2.61743100	-1.26673000	0.18470800
H	-4.57651800	-1.34745500	-1.05142800
H	-4.06155600	0.09343000	-1.96162800
H	-3.92459600	1.94912500	-0.53738500
O	-4.55728200	-2.26160300	1.28205400
H	-5.28952100	-1.63525600	1.17567800
H	-4.84487800	-2.90155200	1.93525700

31

explicit-17_cocarb.xyz

N	2.968514	-0.291721	-1.426220
O	2.573764	1.528752	-0.155605
H	-0.366171	-1.588327	-1.106863
C	0.041981	0.579153	0.614185
C	-1.426604	0.272569	0.632413
C	-1.922145	-0.850737	1.285970
C	-3.276894	-1.160911	1.263826
C	-4.162591	-0.340730	0.576755
C	-3.688011	0.788369	-0.082646
C	-2.335325	1.083011	-0.049725
O	-5.501650	-0.586847	0.518125
H	0.211703	0.613604	-1.526899
H	0.544375	0.083485	1.445205
H	0.215709	1.648983	0.715752
H	-1.240896	-1.489790	1.831554
H	-3.643954	-2.035655	1.785848
H	-4.388349	1.423302	-0.604958
H	-1.977380	1.969159	-0.557973
H	-5.703931	-1.379929	1.022907
H	0.914082	-1.827951	-0.112329
C	4.397636	-0.071558	-1.508865
C	5.100838	-0.421091	-0.200290
O	4.679873	0.285291	0.864579
O	5.941030	-1.269115	-0.101694
H	2.554439	-1.156813	-1.742738
H	4.583579	0.976956	-1.744325
H	4.810352	-0.696691	-2.292304
H	4.003094	0.950025	0.580252
O	2.529403	-1.658067	1.566110
H	3.265470	-1.033016	1.611403
H	2.875325	-2.469678	1.945331

31

explicit-17_cocarb2.xyz

N	3.00073200	-0.16127700	-0.69813800
O	2.17911200	1.85615600	-0.12021200
H	-0.24026700	-1.70924000	-1.00078100
C	-0.31266400	0.66819400	0.55306900
C	-1.74388200	0.25995000	0.36353700
C	-2.29919600	-0.80079700	1.07022400
C	-3.61192400	-1.20458400	0.85591500
C	-4.39326900	-0.54341000	-0.08278200

C	-3.85734900	0.52164000	-0.79991700
C	-2.54850700	0.91127900	-0.57293400
O	-5.68604600	-0.88639400	-0.33997500
H	0.21291600	0.45967100	-1.51470400
H	0.05757900	0.30990100	1.51651900
H	-0.21257100	1.75188900	0.55364200
H	-1.70422300	-1.31668300	1.81207500
H	-4.02772400	-2.02796500	1.42276000
H	-4.47847700	1.03395700	-1.51968300
H	-2.14401800	1.74707100	-1.12914900
H	-5.94270300	-1.62008200	0.22625700
H	0.73356600	-1.75291300	0.30001300
C	4.37901100	0.28099600	-0.67037700
C	4.87647600	0.44774200	0.76148900
O	4.33183900	1.45167200	1.43553100
O	5.69448600	-0.28862300	1.25924600
H	2.79720300	-1.13865000	-0.85035100
H	4.45807300	1.23627600	-1.18974900
H	4.98804500	-0.46402800	-1.16587000
H	3.60527600	1.85266300	0.89950900
O	4.50081000	-2.61347200	0.08746300
H	4.81445200	-3.51365200	0.18855100
H	5.11018500	-2.05539000	0.59439800

31

explicit-4b_cocarb.xyz

N	0.74153671356611	1.99362970432227	0.66733037140565
O	1.59873089431700	1.98724110142725	-1.43592974011476
H	3.30887473078116	-0.11830267615375	1.97277560707235
C	2.40575103450377	-0.71691481280353	-0.81119547447199
C	1.04283624384096	-1.33555176287377	-0.67005424527910
C	0.82303914676810	-2.41782533959521	0.18118546122510
C	-0.45551874908602	-2.89689920834697	0.43395381828006
C	-1.54994270682387	-2.29135756182229	-0.17039862420743
C	-1.34495342751523	-1.24880579143177	-1.07101261194337
C	-0.06452637533800	-0.77764939155448	-1.31138916867461
O	-2.79350708557784	-2.75160234263638	0.13167605222508
H	3.58031740950295	0.89732605831802	0.00220340023713
H	2.56529107685647	-0.35971879005463	-1.82660726022292
H	3.17961329927453	-1.44960431879863	-0.57916593834844
H	1.66800147570182	-2.89452777659475	0.66175074215091
H	-0.62048807358472	-3.72381955142057	1.10907187404784
H	-2.19324790231748	-0.80484439198715	-1.57415210925802
H	0.08151093592343	0.04437706475658	-1.99793212777565
H	-3.42923329574777	-2.03675859767088	-0.01805271648449
H	1.78475254824019	-0.63119635085631	1.67372915767833
C	-0.45896273434045	2.70041277122639	0.32285959643025
C	-1.67132723996852	1.81730188473760	0.52356275820640
O	-1.75400277347902	0.99576921963162	1.41278101240862
O	-2.63349293266536	2.05225557076514	-0.36227364528705
H	0.82445468524847	1.54764352450790	1.56825074762763
H	-0.39033977038927	3.01607507610275	-0.71387043198011
H	-0.59531978046457	3.58930825089765	0.94326655959998
H	-3.37194504733671	1.42908476996371	-0.19654192419225
O	-4.05136252981993	-0.18777175640697	0.54714667696437
H	-3.28970185983003	-0.02762644466711	1.13978407676788
H	-4.83400494366867	-0.21730910667912	1.10409029817718

31

explicit-4c_cocarb.xyz

N	0.123312	-1.400638	-0.593994
O	0.639610	-1.913522	1.543920
H	2.829879	-1.358896	-1.514363
C	2.132201	0.711252	1.009698
C	0.942145	1.527295	0.589603
C	0.979433	2.357524	-0.529231
C	-0.138109	3.063730	-0.945112
C	-1.328188	2.947596	-0.236660
C	-1.387161	2.127595	0.883708
C	-0.257906	1.428177	1.288195
O	-2.401130	3.662708	-0.682373
H	3.005327	-1.236095	0.812817
H	2.078119	0.506434	2.077699
H	3.056343	1.264858	0.829129
H	1.898520	2.452994	-1.090117
H	-0.103302	3.709739	-1.809977
H	-2.310454	2.041561	1.443252
H	-0.313767	0.783190	2.154649
H	-3.146948	3.516901	-0.093207
H	3.297751	0.195265	-1.249742
C	-1.175986	-1.982053	-0.506815
C	-1.152244	-3.492379	-0.594592
O	-0.208083	-4.174290	-0.902519
O	-2.354941	-4.005884	-0.305341
H	0.451361	-0.923259	-1.418730
H	-1.806308	-1.612121	-1.314305
H	-1.652262	-1.717087	0.436829
H	-2.288097	-4.968408	-0.385430
O	2.530209	-3.444335	-1.343707
H	1.592154	-3.656621	-1.215310
H	3.011039	-4.140553	-0.892366

31

explicit-1_nh.xyz

N	-1.90333700	-0.51271500	-0.84503600
O	-1.96090900	-1.11059700	1.32525300
H	0.37674700	-3.39607100	-1.57893100
C	0.69186100	-2.16403200	0.92045100
C	1.49549400	-0.94165100	0.57657200
C	1.07829200	0.32575900	0.98097300
C	1.76238300	1.46605600	0.59056300
C	2.89322300	1.35740500	-0.21228300
C	3.33824100	0.10276400	-0.61122200
C	2.63890300	-1.02871200	-0.21782900
O	3.60441100	2.43937200	-0.62822200
H	-1.00001100	-3.29663600	0.22596300
H	0.28862700	-2.09511500	1.92870000
H	1.32273200	-3.05267900	0.87013500
H	0.20583300	0.43082000	1.60782100
H	1.41136800	2.43935000	0.90870300
H	4.22602600	0.02964500	-1.22173800
H	2.99954500	-2.00190400	-0.52562600
H	3.18205600	3.24284300	-0.30945400
H	0.63072500	-1.79690500	-1.65542000
C	-2.94303700	0.49463500	-0.70482400
C	-2.48429600	1.74393300	0.04851900
O	-2.12654100	1.53734600	1.31784800
O	-2.46931700	2.83393500	-0.45286900

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H -1.61237200 -0.72942400 -1.78968300
H -3.79635000 0.06533100 -0.17599700
H -3.24704600 0.80149200 -1.69880500
H -2.18074600 0.57256600 1.52086900
O -1.53939800 -1.45107400 -3.61298400
H -2.27008400 -1.86530200 -4.07627100
H -1.13770500 -2.12943200 -3.03921900

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explicit-2_nh.xyz

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N 1.53663999791462 0.23921598484667 -0.92074640294330
O 1.49306071676713 0.35467068610166 1.33058301889623
H -0.30730380372139 3.27794907175493 -1.39494032057075
C -0.92879484687189 1.89559080781544 1.09975077328894
C -1.89674968414703 0.82346506256304 0.68698499165286
C -1.67348544674868 -0.51224743542147 1.01905188195530
C -2.53954701326562 -1.50983170680999 0.59566504189109
C -3.65234998426239 -1.18673416419546 -0.17388609576110
C -3.89599855806758 0.13867815839591 -0.51068000261874
C -3.02243295202991 1.12574033309350 -0.07922159691637
O -4.53722987923712 -2.12239517909040 -0.61596825711429
H 0.88440321508099 2.85185102582637 0.47035766120725
H -0.52891726464107 1.68988940301829 2.09086819817612
H -1.43627482368208 2.86015971289394 1.13442137625971
H -0.81190629246998 -0.77107656750142 1.61819188978101
H -2.35449648049909 -2.54111047349352 0.86912765932736
H -4.77029126046470 0.37981865470039 -1.09697846442470
H -3.23010252990018 2.15747954097742 -0.33144250675088
H -4.26434271819621 -2.99236105654888 -0.31004498824794
H -0.92845839992506 1.77108335326405 -1.52230060483741
C 2.36272814610001 -0.94907347226347 -0.94122351477899
C 3.81408054494738 -0.63020593705076 -0.59838479834251
O 4.02559642717409 -0.24181722498100 0.65219945548957
O 4.70941138269991 -0.71009656837346 -1.40488095166664
H 1.37565590833134 0.74154281894771 -1.78309952477223
H 2.32175822581661 -1.38011951489467 -1.93329423976847
H 1.97350042427415 -1.65906838704966 -0.21132055671636
H 3.15949896930756 -0.13701300677365 1.11619834388932
O 3.06853153534526 0.36059116734849 -3.50532358379493
H 3.83861819311476 -0.00393124679763 -3.04314423097351
H 3.41578257676785 0.97207787316569 -4.15708721704277

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explicit-3_nh.xyz

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N -2.04771687764387 -0.63342780068061 -0.86929440110628
O -1.90769790841352 -1.05035014015744 1.33828218057637
H 0.39349750161186 -3.37482939738205 -1.57306359967261
C 0.69936883989010 -2.12732889790985 0.91717837414891
C 1.52880022691881 -0.93216762564198 0.53744465609340
C 2.71159671561517 -1.08245727021556 -0.18077257660753
C 3.45808037740700 0.01783881028492 -0.58653983454743
C 3.02035303304931 1.29939873331665 -0.27661100101120
C 1.84139347092367 1.47156898655953 0.44254305586798
C 1.11162322171661 0.36648714056122 0.84368327560725
O 3.70230182407703 2.41822624775660 -0.64209204347085
H -0.97343966402317 -3.28745673043627 0.22936904871292
H 0.29464847541189 -2.01892771425821 1.92113133699238
H 1.31933327959599 -3.02482620509386 0.90042282818437
H 3.07022963099251 -2.07644587038502 -0.41539246670806
H 4.38135891336234 -0.12201449987185 -1.13440590307214

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H	1.51047247531932	2.47133783240369	0.68141105354843
H	0.20429043410778	0.51838948378481	1.40904722322168
H	4.50054657675244	2.16971263190656	-1.11736681448420
H	0.63891915585969	-1.77380321897414	-1.64737002127273
C	-3.16257830933499	0.29040823007794	-0.73030399169804
C	-2.76651545913704	1.63777375964840	-0.12754788975810
O	-2.26384327276128	1.57637687643506	1.10808534472189
O	-2.91595716352746	2.67653238635679	-0.70896245946936
H	-1.80592979612767	-0.90527233340101	-1.81349032164632
H	-3.92862855101089	-0.16047889196978	-0.09642079771559
H	-3.57063925432154	0.47230814827415	-1.71757065080246
H	-2.22279225954341	0.63468138313663	1.39915536344353
O	-1.88976631007618	-1.78409210994156	-3.52834532778585
H	-1.22126950353875	-2.26430834763101	-3.00450341043881
H	-1.46661980978389	-1.52023240103027	-4.34793208268634

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explicit-4_nh.xyz

N	-0.01043519477338	1.31717853458497	-1.57853858963692
O	-2.05149975211677	1.01929159546734	-0.67502628936585
H	-0.13154062861725	-2.15122773993054	-2.99556229503939
C	-1.37411871687543	-1.77800129654387	-0.51018371822130
C	-0.20731742487037	-1.79151595219257	0.43675685630768
C	-0.02069492390334	-0.76045577825285	1.35656723949823
C	1.10061098111877	-0.71714814182612	2.16984108483494
C	2.06104165922664	-1.71980661258802	2.08323118257093
C	1.88599616756914	-2.76743697986568	1.18707161304528
C	0.76166865753167	-2.79314340546136	0.37505290312251
O	3.18184451489394	-1.73054017822279	2.85344074730298
H	-1.97332093201361	-0.95762901812161	-2.40627789213812
H	-2.27264548412139	-1.41251629114523	-0.01722821834066
H	-1.57519528458511	-2.78799120454714	-0.87038277750878
H	-0.75680143302588	0.02437222914144	1.44218632625436
H	1.22768245373298	0.10027972380496	2.86796907840453
H	2.63060829279102	-3.54815375961186	1.13939642944974
H	0.62979728211167	-3.61877654184415	-0.31258630738011
H	3.19789054635128	-0.94418604827712	3.40747060787985
H	0.83038691158856	-1.50019721715168	-1.86526886119738
C	0.04214932822226	2.73462634790399	-1.25648045978895
C	0.23850336499882	3.01468335234075	0.23397451982173
O	-0.75029691764092	2.58811989253855	1.02270800417107
O	1.19623839828969	3.59604014161133	0.66351714063326
H	0.72462644369093	0.96532927375544	-2.17845020509305
H	-0.88315707776947	3.21540774007618	-1.58015879978228
H	0.88233306814102	3.16659937573415	-1.78758030513015
H	-1.42156922425544	2.11078379409849	0.47814008683132
O	1.82288599177931	0.53366389883727	-3.74669336746119
H	1.72833486733939	0.92618829593051	-4.61681933511352
H	1.16176163075316	-0.17967305227845	-3.67702181033713

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explicit-5_nh.xyz

N	1.50055953304097	0.23770791730438	-0.95990785106465
O	1.51007201277634	0.37491372197145	1.29076062790774
H	-0.34824160883345	3.27700710897543	-1.41508184079608
C	-0.93066227457280	1.89551180855877	1.09295015610310
C	-1.89978934152456	0.81837757395622	0.69639142872961
C	-3.04133017102897	1.11502875194806	-0.04231950082162
C	-3.91580383719188	0.11704818229623	-0.45676026850000
C	-3.65408120785392	-1.20725229568592	-0.13051525848579

C	-2.52182148495126	-1.52417574301902	0.61349195858662
C	-1.65931346434055	-0.52017109888532	1.01862127678724
O	-4.46910215282603	-2.23281967502734	-0.50159074811956
H	0.86799463666677	2.85972046622658	0.43407634477126
H	-0.51491076843055	1.69267794254437	2.07815722585786
H	-1.44176806440575	2.85794334342163	1.13401134376595
H	-3.26459839023425	2.14516033277053	-0.28738143793058
H	-4.80267170786943	0.37039688224027	-1.02369244458432
H	-2.33753128764627	-2.55697007031150	0.87030264004552
H	-0.78302433646165	-0.77180221976836	1.59932649280058
H	-5.21601265617615	-1.88685873908031	-0.99884699291706
H	-0.97537769486125	1.77085020947919	-1.52439343871395
C	2.32677067182733	-0.95045113943577	-0.98849644727546
C	3.78527533399009	-0.62620027879927	-0.68368810518292
O	4.02669141385230	-0.22802035086541	0.55834613479720
O	4.66062949364338	-0.70933737195482	-1.51163010131797
H	1.32005992942614	0.73198544577054	-1.82294571419597
H	2.26245515059663	-1.39119637621577	-1.97506167208486
H	1.95534063913998	-1.65370482208017	-0.24304725857377
H	3.17200237185942	-0.12105763051701	1.04243042307562
O	2.97046592650529	0.33933089687133	-3.58228307969177
H	3.74846208885670	-0.02288166634574	-3.13139432222586
H	3.30703346726035	0.94324613209369	-4.24656493545317

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explicit-6_nh.xyz

N	2.32441408073682	-0.88315252784585	0.16627483299787
O	1.06282562835189	-1.04003247250556	-1.70589442095064
H	-0.30879497255424	-2.42685405696924	2.22252727342378
C	-1.15174495524024	-2.14458219314279	-0.41915141658189
C	-1.94156700227045	-0.87453229635730	-0.25599719608026
C	-2.88920518603502	-0.75568253391002	0.75721258489840
C	-3.60759546975532	0.41885918086437	0.94728921682169
C	-3.38423404322196	1.50394633907996	0.10992207454538
C	-2.44682270437929	1.40410409442712	-0.91273490223511
C	-1.73609289207216	0.22881599773118	-1.08891347477262
O	-4.05489817377989	2.68298360351898	0.23728741030076
H	0.62636004682667	-3.12691767636887	0.26022313403515
H	-0.98994881967579	-2.36145271897000	-1.47274805868495
H	-1.71689935533346	-2.97378060526078	0.00984850178901
H	-3.08539845265369	-1.60057212804563	1.40464109868953
H	-4.34476332910924	0.48568630190967	1.73747922697124
H	-2.28954000718157	2.25297475088634	-1.56181022621642
H	-1.00545582335115	0.15710333095700	-1.88039845715878
H	-4.67365452852338	2.62216691243887	0.97086809019127
H	-0.41654397816817	-0.87455702132548	1.76364984886643
C	3.31287651221561	-0.03257393066970	-0.42373766062476
C	3.41704185269983	1.29516797954517	0.28903121111522
O	4.28959857533910	2.10118257496994	-0.33458980873869
O	2.82860782480897	1.61268605932772	1.29044539321054
H	2.39868942901486	-1.07163241718849	1.15674888540386
H	3.05059346054993	0.14264583767248	-1.46531831201510
H	4.30455846757828	-0.48965137804358	-0.40988011231453
H	4.33569273140121	2.92541110524015	0.17126519610032
O	2.54422275232561	-0.75623617127537	3.12712307016130
H	2.52352219780178	0.17919811197105	2.89360337725049
H	1.66359378164403	-1.09241248119812	2.89290350782681

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explicit-7_nh.xyz

N	2.43689669537575	0.01116176933554	0.80625171748092
O	2.34670884780308	1.69686167512332	-0.70162282121774
H	0.96655722465163	-1.15469326879393	-1.65911688340510
C	-0.54101562005797	0.55749140817879	0.79169854264666
C	-1.96718541839762	0.19347824068597	0.48942901227336
C	-2.81078710386756	1.08328661676399	-0.16979628841439
C	-4.11471313062882	0.73335799965532	-0.49146254183166
C	-4.59580481916799	-0.52739713856096	-0.15485901759650
C	-3.76859226918903	-1.42953577641043	0.50300344201026
C	-2.46811487033070	-1.06622080399504	0.81908372654832
O	-5.86626736436262	-0.92894050374306	-0.44086447436061
H	0.04534525295362	1.07745783146953	-1.21091895193783
H	-0.16743294481772	-0.06200492614028	1.60545862951302
H	-0.47299953868854	1.59935528708083	1.10732156331743
H	-2.44808595613069	2.06878223163570	-0.43150497883666
H	-4.75963978572651	1.44064693636575	-0.99755378433314
H	-4.15757258248554	-2.40246221882680	0.76514005545750
H	-1.82665755580503	-1.76871983051208	1.33451559006281
H	-6.33595495804355	-0.21514223181886	-0.88194819602976
H	-0.62030848908165	-1.21124531955796	-1.25147544996980
C	3.86012692952304	0.11172322156178	0.92755520417869
C	4.57661974079131	-0.59809735991787	-0.20464995050249
O	5.90543272913087	-0.40760323333234	-0.12222792213341
O	4.05336936628520	-1.25900430426927	-1.06023250108739
H	1.99786710370978	-0.84429568066391	1.12709465245227
H	4.18870926869969	-0.32624130706517	1.86879283095104
H	4.16727824058370	1.15504829549282	0.91747222588700
H	6.30979710456348	-0.87842442265742	-0.86495099963913
O	0.88244085299281	-2.43714758072010	1.40085476541687
H	1.25211396241527	-3.31709728750352	1.30099123571346
H	0.62423526234855	-2.13398934493201	0.49747122533518

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explicit-9_nh.xyz

N	2.68352797264641	-0.62499400490038	1.13230822252672
O	2.18237029286849	-1.71897773069004	-0.78951041484374
H	0.33984544357415	-1.23583139820097	2.58479078176634
C	-0.24710372975651	-0.03503388196613	-0.48122075896732
C	-1.72502906899798	0.16179003846246	-0.30673705930228
C	-2.22850941467462	1.26728462033487	0.37209877987225
C	-3.59471013470544	1.42910664780511	0.57050763716461
C	-4.48130839008525	0.47640140580656	0.08517227241310
C	-3.99678637635242	-0.63549339642158	-0.59717267833272
C	-2.63350523729764	-0.78353455184436	-0.78579515315102
O	-5.83023439987203	0.57741004833190	0.24222396985871
H	-0.10639947414217	-2.01162143080887	0.34606882181542
H	0.27284615332656	0.91748453638827	-0.37141595839709
H	-0.01974387778993	-0.42151106465191	-1.47290850043935
H	-1.54561643654253	2.01680203464371	0.74985107987681
H	-3.96837774354054	2.29891072014491	1.09579370999429
H	-4.69819582504884	-1.36394814769743	-0.97630004262670
H	-2.26543640561955	-1.64716828357098	-1.32416019719311
H	-6.03875173526761	1.39020645025282	0.71212443418554
H	-0.92096304310058	-0.37779333122809	2.00388223486765
C	4.03565715112460	-0.38128112473171	0.72144338559329
C	4.15267460078609	0.88438719635188	-0.10366612562465
O	5.38849367149443	1.02361766876912	-0.60079613284705
O	3.27128288148831	1.68429856827931	-0.28707987645714
H	2.30187937816797	0.00578570966473	1.82150124262848

H	4.39645669011792	-1.21431279720849	0.12358171886703
H	4.68538589335847	-0.27982465886562	1.58960079591385
H	5.41030174180306	1.85179236264919	-1.10219549698603
O	1.50685172881646	2.01276595835523	2.17552135155762
H	0.85658440726494	1.29391463630236	2.10320415807084
H	1.87232374134418	2.12316478630027	1.28976210021799

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explicit-11_nh.xyz

N	-2.43203535186263	0.22741157127222	-0.24196215726539
O	-2.12156303251155	2.16468869894144	0.90199932683409
H	-0.61581682551435	-0.36524595559336	2.39314882617034
C	0.50749817908334	0.48659689179766	-0.64016193563413
C	1.95051624885938	0.12806504664876	-0.42404156068777
C	2.89930280144908	1.10670822184361	-0.14085218629796
C	4.22400231762654	0.77378349118990	0.10388502088292
C	4.62044307113969	-0.55902129216115	0.07008345667779
C	3.68795224882240	-1.55035019111241	-0.21047759061438
C	2.36790552400133	-1.20287198859010	-0.45495576393857
O	5.90550638002000	-0.94863979929885	0.29929063246059
H	0.22008142361040	1.55929412368767	1.20022807114947
H	0.01421160088153	-0.30804861040123	-1.19762151682362
H	0.42669803137682	1.40397267792323	-1.22458333767429
H	2.60268656515661	2.14716230725313	-0.11663027670396
H	4.95038001826967	1.54844547078661	0.31506321130081
H	4.01015488066216	-2.58069490471129	-0.24090225680912
H	1.64606769451991	-1.97769079749402	-0.67802370934206
H	6.45000118008751	-0.17457842347641	0.46983694130610
H	0.80375621434564	-0.74156487840086	1.68135526217908
C	-3.84699057253939	0.39595324336238	-0.38877372865447
C	-4.61745095725635	-0.77242304440353	0.17603694572230
O	-5.93939481342022	-0.56904053092178	0.06409894944684
O	-4.14343409040994	-1.77256299976875	0.65013717872713
H	-2.03673719360933	-0.68201594812111	-0.46194790485268
H	-4.14317844281035	0.50908154367657	-1.43424283900665
H	-4.14766664827353	1.30579323765443	0.12857349090706
H	-6.38427322679845	-1.35053389784120	0.42270010080521
O	-1.27373417083309	-2.45724981574216	-0.23984746346775
H	-2.11616915838677	-2.76656841731418	0.11039940986537
H	-0.85984928986195	-1.96475101175626	0.50027699292485

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explicit-16_nh.xyz

N	-2.30174400	-0.97633900	-0.21993600
O	-2.08069400	1.25829100	-0.45155900
H	-0.28457900	-1.17476400	1.96308700
C	0.73344900	0.13010500	-0.92753600
C	2.19236700	0.15429200	-0.57316900
C	2.98728300	-0.97917300	-0.70475700
C	4.32842400	-0.96632900	-0.33825800
C	4.89400500	0.19585700	0.16928300
C	4.11506400	1.34141300	0.30610400
C	2.78173900	1.31218500	-0.06213700
O	6.20003000	0.27791500	0.54435800
H	0.02640700	0.92749000	0.93215200
H	0.51729900	-0.72947200	-1.56377600
H	0.45522300	1.03173300	-1.47176200
H	2.55742700	-1.88675400	-1.10733400
H	4.93272300	-1.85716900	-0.45338300
H	4.57016700	2.24057600	0.69428400

H	2.18550100	2.20923200	0.04196900
H	6.63307700	-0.56690100	0.39053200
H	1.06030400	-1.40424300	1.06829700
C	-3.66135100	-0.99945700	-0.71751800
C	-4.64246900	-0.45212600	0.31359300
O	-4.53462300	0.84550000	0.56317000
O	-5.45238800	-1.14816300	0.87834100
H	-1.90722100	-1.81938100	0.17282900
H	-3.92675000	-2.02442700	-0.94269500
H	-3.71951300	-0.39212200	-1.62102900
H	-3.74515600	1.20916800	0.09274800
O	-3.57970000	-3.29275300	1.18453100
H	-3.65287700	-3.97699500	1.85196000
H	-4.40267100	-2.78231400	1.22985800

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explicit-17_nh.xyz

N	2.73965766885761	-0.48994509222625	-0.94044561017487
O	2.11929246036445	1.31247538314124	0.25431942581862
H	-0.80846968533840	-1.76790179777685	-0.61557079142792
C	-0.50576383987841	0.56759797219882	0.55128528679270
C	-1.96768876092934	0.29103949560584	0.35056937181737
C	-2.63507328354930	-0.67384754094204	1.09765008328425
C	-3.97870157745925	-0.95729936656717	0.87935989935038
C	-4.67827105260125	-0.26965829488703	-0.10366464321301
C	-4.02959758075098	0.70080211870836	-0.86177305498354
C	-2.69211009316223	0.97087864215700	-0.63085133092202
O	-5.99407069584684	-0.49511990854766	-0.36799789972519
H	0.03767127346360	0.28542104962512	-1.50310311964870
H	-0.18087491200159	0.20579717121613	1.52825236769569
H	-0.30619382219188	1.63669037218050	0.52893074820826
H	-2.10423242202084	-1.20585672718853	1.87604043771752
H	-4.48141599938865	-1.70558483935136	1.47878771930212
H	-4.58779695156611	1.23549839339691	-1.61594902298895
H	-2.20071244133560	1.73519239498154	-1.21886808298522
H	-6.33382051484238	-1.16590073038503	0.23166041627017
H	0.54247742982189	-1.98458892885845	0.25929764660050
C	4.14018726617216	-0.10058221941987	-0.99175898074363
C	4.88351216495201	-0.28586043575553	0.33042243323350
O	4.38356158080731	0.39504296205245	1.36344377132543
O	5.86062794290235	-0.97525086161525	0.42956259392092
H	2.46794903297323	-1.29064987025410	-1.49549534484036
H	4.21194157234690	0.94971466955327	-1.28135843667529
H	4.63287790444901	-0.71565559334734	-1.73564247842534
H	3.59844111839913	0.91241255701795	1.07272045936975
O	1.78579800231579	-2.63672925728627	-2.61902198683658
H	1.56601063936542	-3.28358598279238	-3.28992890306872
H	0.99548245711863	-2.46973184765864	-2.07036400279814

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explicit-4b_nh.xyz

N	0.64343169639010	2.20839740778698	0.87232928644165
O	1.10684295661675	1.86034367139994	-1.29951756041279
H	3.00301277997053	-0.51671407803311	1.87017228636402
C	2.15766656044807	-0.71038475999979	-0.74377508899103
C	0.93738929565798	-1.55330264985141	-0.49184745088529
C	1.04374879696483	-2.80113952830508	0.12179577231195
C	-0.07556383812581	-3.56512033942230	0.41912223926413
C	-1.33805156569231	-3.07575288199275	0.10912059457279
C	-1.46672991249481	-1.83276746808329	-0.50028509510010

C	-0.33918586544305	-1.08421101360726	-0.80048889456205
O	-2.41272060031015	-3.85292008802148	0.42509115225679
H	3.25397745428177	0.92674928747921	0.11042335281857
H	2.14858120688290	-0.29660923237385	-1.75007638564238
H	3.05153986388871	-1.32800322732788	-0.64229047471739
H	2.02440546775489	-3.19010939915044	0.36446091659553
H	0.01391763470490	-4.53473476118477	0.88640223095104
H	-2.44806442376947	-1.43883908546359	-0.73202016749032
H	-0.45976140319379	-0.11911587116066	-1.26800844333209
H	-3.21858307071530	-3.40178221506608	0.15683337129990
H	1.38979962323117	-0.57566312333703	1.75443801135271
C	-0.25581154871241	3.27680287330081	0.55429934111863
C	-1.58606473894807	2.79175564550525	0.01601268486725
O	-1.97780060276405	1.65789881837457	-0.00499423524923
O	-2.31061819438779	3.83518493294083	-0.43191881862746
H	0.82909550274145	2.00904705323249	1.84386572876048
H	0.17724330182750	3.93929934504153	-0.19382905557844
H	-0.44906824048131	3.86156176973981	1.45220475891440
H	-3.15058964974439	3.48074774395184	-0.75606484499866
O	1.58581250911147	1.95840228555898	3.65067096020949
H	1.97916905631330	1.23417513997050	3.12204706497660
H	1.19663579257577	1.54851361414141	4.42578601316802

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explicit-4c_nh.xyz

N	-0.23972371798349	-1.46705315135087	-0.72776430962209
O	0.41235848114554	-1.46337567196845	1.43970080023515
H	2.90060805109458	0.23543222960246	-1.74541372671902
C	1.98126152600563	0.87347846667172	0.80821237074289
C	0.90821618726711	1.88661842811488	0.52903676946063
C	1.12716071345641	2.94750225835275	-0.34941216031266
C	0.12730755889841	3.85954211931460	-0.65328443852834
C	-1.12574475384105	3.72078793228152	-0.07034102486320
C	-1.36425293076482	2.67328652148895	0.81314098236896
C	-0.35534807009047	1.76766314121456	1.10624598479188
O	-2.07714837784156	4.64053756152253	-0.39337469930363
H	2.69474006538185	-1.04041891690421	0.15447485975952
H	1.93146672494644	0.53675289914821	1.84186985733895
H	2.96422134789285	1.31862183889104	0.64632695589472
H	2.10561114127872	3.07437018698418	-0.79431707578380
H	0.30502062209313	4.68371485217495	-1.32815453016880
H	-2.33788057540204	2.56933459969306	1.27554415718580
H	-0.54815469940264	0.95493061471184	1.79241078856056
H	-2.88997721140136	4.43981045434249	0.07973533764401
H	1.33689608134087	0.67315917734281	-1.77090745347768
C	-1.30269203417291	-2.39596398589403	-0.48086696845027
C	-0.85546195562514	-3.83474349771803	-0.63609466663597
O	0.20631561581875	-4.19949228928218	-1.07003536110451
O	-1.81985999547548	-4.68015841938313	-0.24485163058019
H	0.08875914758980	-1.40203710925404	-1.68126105980480
H	-2.12371726579384	-2.22624564962952	-1.17667340056629
H	-1.68056839735824	-2.26240779803530	0.52956291259293
H	-1.49142785569016	-5.58030408276125	-0.38431190385553
O	1.06891989806119	-2.29720180082730	-3.26285138625271
H	1.63483111435790	-1.64493130222209	-2.81918613451340
H	1.08657237665882	-3.07679365448227	-2.69510961972555

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explicit-1_nh2-1.xyz

N	-1.42592146525004	0.38334069097923	-1.17146603435542
O	-2.22105082552598	-0.74123890807494	0.61807620223382
H	-0.14360298820418	-2.48149850334933	-2.77277504810128
C	0.02605899345768	-2.54661273727562	0.20619846608906
C	1.20707087326900	-1.67816730963049	0.53781238042921
C	1.06360475154813	-0.54854686716195	1.34274934748201
C	2.12961473343756	0.30491993000356	1.58081807395895
C	3.37343628662655	0.03700100076871	1.01875684395312
C	3.54381076053613	-1.09192935796099	0.22735157872164
C	2.46548297877335	-1.93326362392474	-0.00666026933152
O	4.45576951075251	0.83939731501587	1.21594701178392
H	-1.61690595398232	-2.67433910222531	-1.16798247155188
H	-0.61307637635845	-2.67833972130600	1.07763278536731
H	0.36713707772844	-3.53077923935722	-0.11581960883637
H	0.10675308430502	-0.32707122333585	1.79109791128820
H	1.99012247399875	1.18081942812992	2.20155562857342
H	4.51745149517036	-1.29729718464002	-0.19254275069248
H	2.60921626404202	-2.81444333849408	-0.61862707406215
H	4.20112282049222	1.59007374065383	1.76087642839409
H	0.87204590598773	-1.47172746548030	-1.96041525399691
C	-2.12243459030367	1.62260042616864	-0.88696923968444
C	-1.56863353326825	2.36940406519842	0.32758209019175
O	-1.62689906928042	1.69680290714282	1.47727504185155
O	-1.13719017518611	3.48754978792969	0.25672436207544
H	-0.88447415550611	0.26525727053122	-2.01652278952636
H	-3.17778597892679	1.40851034684932	-0.70479614650432
H	-2.03220047948339	2.27716975214877	-1.74603425654796
H	-1.99289756266482	0.79150707608461	1.31747625857602
O	-1.18847643033720	-4.24761735641315	-3.35668426646844
H	-0.98545948385667	-5.18391068993600	-3.29691069587093
H	-1.91969689843047	-4.17867185670361	-3.97508698737563

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explicit-2_nh2-1.xyz

N	1.60515800	0.04990400	-0.90088800
O	1.47280200	0.55932400	1.29401200
H	-0.19579300	2.86103600	-2.00753400
C	-0.98531500	1.95736800	0.70560400
C	-1.91817500	0.80012100	0.48632200
C	-1.66729300	-0.44432300	1.06354100
C	-2.50016200	-1.52720200	0.82178600
C	-3.60690200	-1.38395200	-0.00866600
C	-3.87802700	-0.15146600	-0.58865500
C	-3.03742700	0.92295200	-0.33685800
O	-4.45976100	-2.41068800	-0.28047300
H	0.81005700	2.83472600	-0.06212700
H	-0.61114200	1.95714200	1.72773800
H	-1.51357900	2.89621700	0.53866400
H	-0.81097300	-0.56302100	1.71240000
H	-2.29428500	-2.48413400	1.28503700
H	-4.74750000	-0.04795200	-1.22086000
H	-3.26621700	1.88396900	-0.77890500
H	-4.17115400	-3.19963600	0.18762000
H	-0.97256600	1.41731100	-1.82680200
C	2.42330700	-1.13293100	-0.72391700
C	3.86812200	-0.83721700	-0.32079300
O	4.01071400	-0.13011100	0.79896600
O	4.80611100	-1.23616500	-0.95570500
H	1.31489500	0.36277700	-1.81682000

H	2.44630200	-1.68435400	-1.65676700
H	1.97551600	-1.75761000	0.05179000
H	3.12547500	0.09408700	1.17482700
O	0.64574400	4.82776900	-1.80912300
H	1.53280000	4.90440500	-2.16913600
H	0.35304700	5.72700900	-1.64476600

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explicit-3_nh2-1.xyz

N	-1.89331100	-0.58759000	-0.94163400
O	-1.80775600	-1.24491900	1.21678500
H	0.32735800	-3.07176700	-2.10084900
C	0.89919400	-2.13424900	0.65786200
C	1.65379300	-0.85057700	0.45384700
C	2.82744200	-0.82125100	-0.29330600
C	3.50137900	0.37005600	-0.53755700
C	2.99843200	1.56231000	-0.03305400
C	1.82765300	1.55501000	0.71877200
C	1.17083500	0.36055900	0.95750800
O	3.60909500	2.76253300	-0.23518600
H	-0.70255200	-3.28436700	-0.18036900
H	0.50414900	-2.19270000	1.67069500
H	1.56728500	-2.98235700	0.50604000
H	3.23352600	-1.74570400	-0.68291700
H	4.41800600	0.36949200	-1.11390900
H	1.44527100	2.48676600	1.10837000
H	0.26724200	0.37027300	1.54917700
H	4.40210100	2.63442400	-0.76374000
H	0.87209100	-1.54102100	-1.84106100
C	-3.04199500	0.28325300	-0.78362300
C	-2.74628500	1.55999200	0.00493500
O	-2.29283200	1.36666900	1.24344600
O	-2.93713900	2.65474200	-0.44884000
H	-1.48990700	-0.76613100	-1.85066200
H	-3.83516400	-0.25992900	-0.26501600
H	-3.39277400	0.57724300	-1.76603300
H	-2.20519100	0.39794700	1.42142500
O	0.15338500	-5.20102000	-1.89464100
H	-0.58906900	-5.65991900	-2.29481100
H	0.78393600	-5.88490500	-1.65757600

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explicit-4_nh2-1.xyz

N	0.94595500	-0.39900600	0.76029400
O	1.28861700	-1.73483300	-1.02761400
H	0.24549100	-2.52038300	2.54142400
C	-1.61872800	-2.27794100	-0.21729900
C	-2.10451900	-0.85779200	-0.29304800
C	-1.72004400	-0.04106500	-1.35283700
C	-2.10696200	1.29106800	-1.41332800
C	-2.89588900	1.82846800	-0.40337400
C	-3.29432000	1.02824200	0.66081800
C	-2.89808500	-0.29898300	0.70717900
O	-3.31095800	3.12806400	-0.40677200
H	0.05219100	-3.46407300	0.41139200
H	-1.42114900	-2.65221200	-1.22046800
H	-2.38363400	-2.91918800	0.22641300
H	-1.09651100	-0.44992200	-2.13635000
H	-1.80181500	1.90934700	-2.24853600
H	-3.91334000	1.45589700	1.43572200

H	-3.21077300	-0.91060000	1.54175200
H	-2.99405500	3.56065200	-1.20492900
H	-1.37940800	-2.67199600	2.33703000
C	1.83051100	0.61015500	0.27749900
C	3.28861000	0.25257800	0.46582500
O	4.07941300	1.11388300	-0.18725100
O	3.72011100	-0.65847400	1.12548200
H	0.41075500	-0.29346700	1.60765000
H	1.64834700	1.54776800	0.80086300
H	1.67121100	0.78489000	-0.78627500
H	4.99619400	0.84789200	-0.02570400
O	2.33682200	-2.80635500	2.42936400
H	2.77810100	-2.05288600	2.00608700
H	2.87902800	-3.56831200	2.21696200

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explicit-5_nh2-1.xyz

N	1.61772600	0.04882200	-0.89210500
O	1.50364800	0.57883200	1.29906500
H	-0.13962900	2.87890300	-2.01099500
C	-0.95420600	1.98183500	0.70516200
C	-1.89712600	0.83408300	0.47919300
C	-3.02034500	0.97527800	-0.33014800
C	-3.86966600	-0.09570600	-0.58473000
C	-3.60059500	-1.33680800	-0.02309700
C	-2.48646600	-1.49751300	0.79478700
C	-1.64910000	-0.42249500	1.03892200
O	-4.39162600	-2.42638300	-0.22891700
H	0.84883700	2.84745500	-0.05947700
H	-0.58198200	1.97371200	1.72803700
H	-1.47367100	2.92612000	0.54124000
H	-3.24896100	1.94202500	-0.75942800
H	-4.74261100	0.03790700	-1.21113300
H	-2.29677200	-2.46525700	1.23543100
H	-0.78801200	-0.55200700	1.67952300
H	-5.13014800	-2.18490000	-0.79551500
H	-0.94865400	1.45345100	-1.82391200
C	2.42824700	-1.13864900	-0.71005200
C	3.87788800	-0.84778600	-0.32139700
O	4.03357800	-0.13333700	0.79211500
O	4.80868900	-1.25466100	-0.96184000
H	1.32525700	0.35624100	-1.80902100
H	2.44008600	-1.69896700	-1.63778200
H	1.98180100	-1.75290100	0.07460500
H	3.15282400	0.09778200	1.17395800
O	0.84146600	4.79085400	-1.85336300
H	1.73761500	4.75421600	-2.19690900
H	0.66858700	5.71800000	-1.67512500

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explicit-6_nh2-1.xyz

N	1.41273900	-0.32109400	0.62359300
O	1.17640500	-1.46632100	-1.31435900
H	-0.89879900	-2.65629900	2.35669700
C	-1.44199100	-2.22135400	-0.34759600
C	-2.15797200	-0.90112800	-0.33460200
C	-3.19823200	-0.65387900	0.55594300
C	-3.82966700	0.58359300	0.60697100
C	-3.42142700	1.60036900	-0.24634000
C	-2.38715400	1.37155500	-1.14832500

C	-1.76648900	0.13496700	-1.18680500
O	-3.99803700	2.83437100	-0.25094300
H	0.28117600	-3.20471900	0.46716500
H	-1.15730200	-2.49335400	-1.36223800
H	-2.09675300	-3.00377800	0.03938700
H	-3.53676100	-1.44418600	1.21325700
H	-4.64233800	0.75288200	1.30199300
H	-2.08710800	2.16851400	-1.81268500
H	-0.96312200	-0.03777200	-1.88929200
H	-4.70163800	2.86274700	0.40398100
H	-0.97254600	-1.07260600	2.00512700
C	2.54496600	0.40975500	0.13566100
C	3.85169700	-0.30642200	0.40627400
O	4.87058900	0.30582300	-0.21309500
O	3.99014500	-1.28112300	1.09918200
H	1.31190700	-0.38211800	1.62702100
H	2.59739100	1.38795400	0.61259200
H	2.45170700	0.55986500	-0.93679800
H	5.67959400	-0.17660300	0.01131200
O	2.05588900	-1.14360000	3.40985400
H	1.27409900	-1.63492500	3.11117200
H	2.78054300	-1.45894200	2.85632600

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explicit-7_nh2-1.xyz

N	2.38060000	-0.37852200	0.46041500
O	2.04465800	1.47970800	-0.79349300
H	0.46661100	-1.87807100	-1.26718300
C	-0.66971500	0.64773000	0.56736600
C	-2.13260500	0.36395100	0.38041000
C	-2.86690200	1.03350200	-0.59541400
C	-4.20798200	0.75054000	-0.80717400
C	-4.84198100	-0.21979900	-0.03774000
C	-4.12821300	-0.89817400	0.94154600
C	-2.78776800	-0.60224100	1.14187500
O	-6.15649600	-0.54056700	-0.19761200
H	-0.11558400	0.36136900	-1.48428000
H	-0.34263000	0.29070400	1.54494000
H	-0.48168700	1.72030800	0.52069700
H	-2.38467700	1.79217800	-1.19763700
H	-4.76401500	1.28561000	-1.56670800
H	-4.63271600	-1.64475900	1.53688300
H	-2.23943100	-1.13054900	1.91050500
H	-6.53407800	-0.00380400	-0.90047100
H	-0.86900500	-1.75593500	-0.31778600
C	3.75015800	-0.08371700	0.73344800
C	4.70882800	-0.59079000	-0.32176700
O	5.97345200	-0.29512000	0.00853700
O	4.41790800	-1.18721200	-1.32651900
H	1.97818000	-1.28062800	0.66688900
H	4.05168300	-0.50605900	1.69114700
H	3.88113300	0.99628500	0.79226600
H	6.54584900	-0.62751800	-0.69824900
O	1.95363200	-1.15760800	-2.82648100
H	2.79281700	-1.26233100	-2.35496800
H	1.90545200	-0.21450500	-3.00624400

31

explicit-9_nh2-1.xyz

N	2.67196100	-0.39873300	0.98820700
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O	2.10658700	-1.94898700	-0.57133100
H	0.48669700	-0.87701800	2.70003800
C	-0.26463600	-0.05892100	-0.45394000
C	-1.73484900	0.20041500	-0.29311100
C	-2.21569500	1.46883300	0.00890300
C	-3.57856100	1.70953500	0.16644700
C	-4.48628900	0.66705900	0.01865500
C	-4.02324200	-0.61181500	-0.28031900
C	-2.66489600	-0.83162500	-0.43461100
O	-5.83050300	0.83172900	0.15568400
H	-0.15449600	-1.91317000	0.62854600
H	0.28031500	0.88538000	-0.47543700
H	-0.07259800	-0.57128900	-1.39644800
H	-1.51763300	2.28634000	0.12492400
H	-3.93226400	2.70773500	0.39217900
H	-4.73911000	-1.41128600	-0.40403400
H	-2.31786800	-1.82659800	-0.68062200
H	-6.02703200	1.75706300	0.32993200
H	-0.77356900	-0.02396300	2.14556300
C	4.01672100	-0.27406500	0.51640300
C	4.14185200	0.72970900	-0.61195400
O	5.40198500	0.75834700	-1.08354800
O	3.25886600	1.42470000	-1.03346300
H	2.26244100	0.32806500	1.55618400
H	4.36078100	-1.23811700	0.14772300
H	4.68176900	0.03228300	1.32279100
H	5.42620700	1.41125800	-1.79768100
O	-2.79818200	0.00454300	2.96634000
H	-3.21788300	-0.82610700	2.72754100
H	-3.09323700	0.61672400	2.28231600

31

explicit-11_nh2-1.xyz

N	-2.30504300	-0.33116900	-0.11771400
O	-1.85622400	1.62892000	0.92914900
H	-0.27320400	-1.69579100	1.58704900
C	0.73531700	0.63422000	-0.55566100
C	2.20588500	0.34530000	-0.45846600
C	3.02130400	1.08888800	0.39116700
C	4.37246800	0.80493000	0.52216100
C	4.93473200	-0.24130100	-0.20226700
C	4.13940900	-0.99436100	-1.05610000
C	2.78993100	-0.69642900	-1.17701700
O	6.25497000	-0.56710400	-0.11730400
H	0.34233400	0.54515200	1.55059800
H	0.32862400	0.19512400	-1.46773800
H	0.56091700	1.70946000	-0.59316300
H	2.59518800	1.90675700	0.95712900
H	4.99182500	1.39787800	1.18335000
H	4.58838300	-1.79991400	-1.61809700
H	2.17757300	-1.28358000	-1.84846400
H	6.69171300	0.02447900	0.50235700
H	0.98428700	-1.68111700	0.52943700
C	-3.68977700	-0.04312600	-0.30900600
C	-4.56687100	-0.44889800	0.85527500
O	-5.85245900	-0.17337000	0.59627300
O	-4.20156600	-0.95724400	1.88392400
H	-1.92682600	-1.25422200	-0.27054100
H	-4.06733300	-0.53903100	-1.20233700

H	-3.81774400	1.02999100	-0.44737000
H	-6.37016700	-0.43785800	1.37067900
O	-1.62905000	-0.81130700	3.18367600
H	-2.50212300	-0.95114900	2.78911800
H	-1.56378400	0.14400900	3.26842600

31

explicit-16_nh2-1.xyz

N	-2.50204600	-0.77893300	-0.18251000
O	-2.11238400	1.43971400	-0.36684900
H	-0.65328500	-1.18761000	1.98064800
C	0.59757400	0.09876500	-0.83778100
C	2.05976200	-0.00821400	-0.51011600
C	2.80536800	-1.11615500	-0.89284900
C	4.15837500	-1.22183800	-0.58027400
C	4.78569500	-0.20278400	0.12737400
C	4.05294200	0.91472700	0.52105000
C	2.71002600	1.00360900	0.19932100
O	6.10223100	-0.23922600	0.46617700
H	-0.05333100	0.91396200	1.03822000
H	0.30937600	-0.72205000	-1.49605400
H	0.39513300	1.03387000	-1.36036900
H	2.32721400	-1.91656300	-1.44046400
H	4.72234700	-2.09129300	-0.89326600
H	4.55413800	1.70434100	1.06131100
H	2.15514900	1.88228500	0.50044000
H	6.50838600	-1.03531600	0.11012400
H	0.77202600	-1.46146400	1.26713900
C	-3.81846700	-0.74493500	-0.79282000
C	-4.89428300	-0.10709100	0.08651400
O	-4.64789200	1.14558300	0.46716600
O	-5.90058500	-0.68708300	0.38966300
H	-2.08261200	-1.65283000	0.09969100
H	-4.12821300	-1.76122200	-1.00693000
H	-3.76313900	-0.18052400	-1.72597900
H	-3.77981600	1.44673200	0.10960400
O	2.60479000	-1.85271600	2.33200100
H	3.18398800	-1.70215300	1.57607500
H	2.86638000	-1.18912900	2.97502200

31

explicit-17_nh2-1.xyz

N	2.71051700	-0.63213400	-0.72880900
O	2.01235600	1.47929100	-0.33594200
H	-0.50968200	-1.99669400	-1.16273100
C	-0.48777600	0.41298000	0.55997000
C	-1.95529600	0.13767400	0.42137300
C	-2.57603400	-0.88941300	1.12368800
C	-3.92165700	-1.18331800	0.94129600
C	-4.67499900	-0.44222100	0.03949300
C	-4.07602700	0.59605800	-0.66955900
C	-2.73236200	0.87749100	-0.47101900
O	-5.99550400	-0.67949700	-0.19128400
H	-0.07431300	0.13282500	-1.52681000
H	-0.11905400	0.01967500	1.51050400
H	-0.29229600	1.48358900	0.55737300
H	-2.00319000	-1.47197200	1.83237600
H	-4.38383900	-1.98689900	1.50019300
H	-4.67529100	1.17738200	-1.35499000
H	-2.27735100	1.68836800	-1.02427600

H	-6.30125900	-1.38857300	0.38222000
H	0.19358300	-2.06655400	0.31717500
C	4.11211000	-0.29246900	-0.88262700
C	4.80345100	0.08757000	0.42668400
O	4.25704700	1.11189100	1.08019800
O	5.78346500	-0.48124100	0.82364500
H	2.37435600	-1.57174800	-0.88703400
H	4.20157000	0.55065200	-1.57112700
H	4.63434600	-1.14800400	-1.29484500
H	3.46999500	1.44800900	0.58911000
O	-2.20024200	-1.77523500	-2.31583100
H	-2.73828400	-2.26209900	-2.94352900
H	-2.80289600	-1.18052100	-1.85435300

31

explicit-4b_nh2-1.xyz

N	0.64847600	2.10319400	0.92692200
O	1.31673100	1.81698000	-1.21109600
H	2.83729100	-0.35180600	2.26952900
C	2.21916300	-0.83651900	-0.52582400
C	0.95086200	-1.63526700	-0.41023400
C	0.93370900	-2.86227400	0.25167700
C	-0.23966400	-3.58360300	0.42057800
C	-1.43250700	-3.07079100	-0.07158500
C	-1.43882400	-1.84703500	-0.73100500
C	-0.25758900	-1.14159300	-0.90000700
O	-2.56606200	-3.80615700	0.12054300
H	3.27020400	0.76791300	0.41886800
H	2.33934400	-0.44339100	-1.53426200
H	3.07321600	-1.47900000	-0.30835000
H	1.85971400	-3.26569900	0.64058800
H	-0.24535400	-4.53656900	0.92896800
H	-2.36865500	-1.43425600	-1.10117800
H	-0.28067400	-0.18843500	-1.40651200
H	-3.31395200	-3.33471400	-0.25769700
H	1.28656500	-0.72142200	1.89187700
C	-0.24166400	3.17097800	0.60146400
C	-1.56318700	2.70199400	0.02563400
O	-1.94018600	1.56740300	-0.06567800
O	-2.29491700	3.76249800	-0.37183200
H	0.72085000	1.71592600	1.85460600
H	0.21731200	3.82574900	-0.13829200
H	-0.45420500	3.76714800	1.48765900
H	-3.12519500	3.41741800	-0.72933700
O	4.99804200	-0.62520600	2.07051500
H	5.47611300	-1.33765800	1.63997400
H	5.66920700	-0.01773400	2.39006900

31

explicit-4c_nh2-1.xyz

N	0.47438800	-0.93828800	-0.76324300
O	1.18895100	-1.43417400	1.32027200
H	3.07017700	-0.36064400	-1.81152800
C	2.16697200	1.43142400	0.85577400
C	0.82993000	2.04115100	0.54083400
C	0.65723400	2.92031900	-0.52670000
C	-0.58876500	3.43571000	-0.84681900
C	-1.69783900	3.07296100	-0.09180900
C	-1.54813200	2.19991000	0.97895600
C	-0.29248800	1.69389900	1.28762800

O	-2.90333300	3.60645400	-0.44311300
H	3.35543400	-0.31786800	0.50643600
H	2.21212100	1.17090000	1.91197500
H	2.96766900	2.14835200	0.66087400
H	1.51203700	3.20726500	-1.12292500
H	-0.71706600	4.12057600	-1.67206200
H	-2.40867500	1.92211800	1.57500500
H	-0.18474900	1.00641800	2.11564100
H	-3.57729200	3.29981700	0.17037700
H	3.26354600	1.23987900	-1.48475500
C	-0.69257100	-1.74927200	-0.64212700
C	-0.39702800	-3.22705300	-0.77819800
O	0.63433200	-3.71520900	-1.16477000
O	-1.46339900	-3.96081400	-0.43482400
H	0.66402100	-0.37489000	-1.57706400
H	-1.41337100	-1.48321000	-1.41408100
H	-1.16847700	-1.59815900	0.32643300
H	-1.22609800	-4.89221400	-0.55104600
O	3.14600900	-2.46731700	-1.75728100
H	2.27568300	-2.85559000	-1.57449400
H	3.78214200	-3.10775900	-1.43377200

31

explicit-1_nh2-2.xyz

N	-1.54762617997990	-0.95255313336185	-0.93666880895159
O	-2.00600870360063	-0.97954633179759	1.27409130940881
H	0.06254810843441	-4.14841218265121	-0.84636281668913
C	0.67087493426552	-2.23635035288107	1.38906993845940
C	1.49890646176683	-1.12210945821019	0.81290380335976
C	1.13077596729817	0.20583894816731	1.02334768396030
C	1.79717462706811	1.24963814080315	0.40308564320535
C	2.87309971582551	0.98132734576497	-0.43723087496266
C	3.27858691229440	-0.33363042197937	-0.64015762674261
C	2.59298789448123	-1.36854357732511	-0.01615769650726
O	3.56133980780125	1.96033713105068	-1.08393146734512
H	-1.06751120926922	-3.42159785683413	0.93417209501283
H	0.23766016769105	-1.93248539939446	2.34035386730186
H	1.28389104325402	-3.12156931226010	1.56093096357564
H	0.29745366592467	0.43044155058849	1.67100404857143
H	1.46902778169406	2.26845618124166	0.56203646316096
H	4.13019751039141	-0.52870754586396	-1.27540351777767
H	2.93008129423856	-2.38572787089176	-0.16876905643112
H	3.16582824143631	2.81523586907468	-0.88688720261302
H	0.84586696909881	-2.73730753678356	-1.12368029080427
C	-2.31482442407420	0.24201021472227	-1.21597863387293
C	-1.64698790251858	1.48324600547877	-0.62872462620716
O	-1.74349362829560	1.60206893118631	0.69085700388115
O	-1.05985248227086	2.29430516116836	-1.30257795389049
H	-0.96200885414152	-1.32581394917158	-1.66863702228313
H	-3.31579307837848	0.13709271824488	-0.79722266978203
H	-2.37833059333947	0.36233052436183	-2.29099741193173
H	-2.06457289017107	0.74470419953758	1.06838371679233
O	0.46839370459260	0.19450901439972	-2.77204793414174
H	0.11228523204780	1.05306278625089	-2.50508511358107
H	1.32385128470690	0.13954290113429	-2.33366375721360

31

explicit-2_nh2-2.xyz

N	1.63943925697524	0.21412854484536	-0.84827454646697
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O	1.52699074795479	0.38597266762313	1.39708841188520
H	-0.09156860338368	3.34188881248297	-1.42189996144545
C	-0.84284811914618	1.97720170379144	1.00450617118871
C	-1.80539831552363	0.92795907096280	0.52658683210550
C	-1.61200991103029	-0.41869602944607	0.83381100682764
C	-2.46604216587552	-1.39813553287180	0.33989705923631
C	-3.54355346586140	-1.04108278724537	-0.46652651305119
C	-3.75666546028148	0.29696210152619	-0.77634440759287
C	-2.89273894193242	1.26148351414631	-0.28032082064123
O	-4.41266860798941	-1.95375212528427	-0.98075135573544
H	1.03447753618295	2.88598830856558	0.51412100854391
H	-0.51674897378380	1.76277438976976	2.02071600251497
H	-1.33124224506989	2.95197490123441	1.00543861098128
H	-0.78214590434433	-0.70408254229109	1.46490688691068
H	-2.30307033377126	-2.43794879061455	0.59429213640113
H	-4.60243012649779	0.56473878592326	-1.39237814012407
H	-3.07150931989108	2.30043945575812	-0.52248343891196
H	-4.19667553119847	-2.83042671356157	-0.64868385919292
H	-0.56313797953382	1.78430065047854	-1.67447671799515
C	2.26530322712538	-1.09354012249020	-0.85589076719719
C	3.72828811695701	-1.09374147407552	-0.41340404245555
O	3.95655309410861	-0.57984975168813	0.79442269149242
O	4.60345818466214	-1.55417097621478	-1.09412422336381
H	1.36926662085161	0.64439674738982	-1.71948187328511
H	2.21779159797972	-1.48907686378082	-1.86332853729224
H	1.71205236836148	-1.75460896661168	-0.18462584597354
H	3.11000521571485	-0.27604426290259	1.19974973895515
O	-0.80053397072470	-0.36732378845617	-2.51390747556712
H	-1.44820690654212	-0.53673787326888	-3.20263982694822
H	-1.21587228807416	-0.68231813209780	-1.70198901289038
31			
explicit-3_nh2-2.xyz			
N	-1.64513093561856	-0.83159140452095	-0.97544095352812
O	-2.00306688022680	-1.10872812874736	1.23683506129266
H	0.15496432189208	-3.88377086127140	-1.28476725899537
C	0.74627627638415	-2.17954522600480	1.15169098566546
C	1.54824729130332	-1.01442430457978	0.64259157522562
C	2.68346882469032	-1.20305445125076	-0.14119480588241
C	3.37657451191854	-0.12607512549428	-0.68336396906806
C	2.93935118332765	1.17109952369968	-0.43967227323331
C	1.80965159868119	1.38134716415407	0.34723637686318
C	1.13421205416903	0.29789591223907	0.88246467682292
O	3.57054035208535	2.26778286704692	-0.93760550356475
H	-0.91855708618899	-3.42551294562848	0.61007087030711
H	0.31031953595568	-1.94828584866764	2.12195428691144
H	1.38646787004286	-3.05456251315529	1.26680293686009
H	3.04727299131146	-2.20589208668296	-0.32344429472538
H	4.26092132813403	-0.29508790556415	-1.28434877195125
H	1.47261073274104	2.39091607027120	0.53075969982052
H	0.26422183509126	0.47933446205485	1.49550306962043
H	4.32299576469263	1.99592701692188	-1.47159257326914
H	0.91131117098241	-2.43296054008534	-1.38876749126270
C	-2.53466590495266	0.30156736592027	-1.11383014306780
C	-1.96986968235338	1.55112247056982	-0.44186717752744
O	-1.96413333503231	1.52153341466497	0.88677887675313
O	-1.54879714911813	2.49465979529589	-1.06344186160078
H	-1.06615645321206	-1.09200220944177	-1.75973218265676
H	-3.49983285299456	0.05929082933857	-0.66801538806737

H	-2.66162478053344	0.50927703644814	-2.16957800903921
H	-2.18438793801643	0.60601762167218	1.19358239995121
O	0.24313699830599	0.74130583243977	-2.67669951058271
H	-0.24847708427809	1.52969817033840	-2.40904436656501
H	1.00649064545951	0.73434878847925	-2.09000235704918

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explicit-4_nh2-2.xyz

N	-1.63031255813258	-0.84570187095027	-0.95233475081847
O	-1.99646109493596	-1.05134510408067	1.26612301403010
H	0.03886585655561	-4.00572082676606	-1.17131369837488
C	0.70755496775744	-2.25321003500746	1.17477176484356
C	1.48972651498651	-1.08279043614423	0.64820942385033
C	1.10649611522516	0.21826668290913	0.97010941103854
C	1.72484291067062	1.31807378840052	0.39886251700678
C	2.76637559394319	1.13391324637349	-0.50494447607484
C	3.18755365464088	-0.15379086124576	-0.81935969596392
C	2.55053498029864	-1.24537114084925	-0.24241474882572
O	3.40524332128780	2.17165949701369	-1.11004123580472
H	-1.02693614632457	-3.43854013173170	0.70435418562083
H	0.31031031305289	-2.02907367615156	2.16316561648293
H	1.34306088749592	-3.13563163167359	1.25486874380465
H	0.29870674392213	0.37766313673442	1.66757763561469
H	1.38507964253260	2.31552299097820	0.64506455309877
H	4.01381511547327	-0.28445297099735	-1.50275353555936
H	2.89971524875196	-2.24146562259629	-0.48210888470371
H	3.00568360976441	3.00156467196997	-0.83125999326216
H	0.78332945616118	-2.56125026212075	-1.37328292096097
C	-2.43246798134014	0.34841088839794	-1.10765121714025
C	-1.76574292484050	1.55644123683083	-0.45377994141893
O	-1.80873034471933	1.57199552326328	0.87371188860995
O	-1.22403936052886	2.43008844109508	-1.08634564134006
H	-1.06953144441924	-1.14944843678505	-1.73416509016680
H	-3.41260827567013	0.18862108284784	-0.65808709429485
H	-2.54361640563172	0.54858574084121	-2.16677762316577
H	-2.09643756072401	0.68104548158445	1.19667900544463
O	0.26532348831925	0.49429434414627	-2.78902609344259
H	1.15368579367130	0.44129999370657	-2.42198221760536
H	-0.09658375322627	1.31780897662498	-2.43360340202239

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explicit-5_nh2-2.xyz

N	1.79419004807123	0.22489104459878	-0.93354962252201
O	1.40819823839973	0.15142592001943	1.28741530879843
H	-0.18436544766930	3.16414833910685	-1.50664962103598
C	-0.84581158346803	1.88305781980755	0.96524531493923
C	-1.88367171587978	0.88321158169935	0.54259113645551
C	-3.00121403696600	1.27804230832033	-0.18568313888510
C	-3.95646751558046	0.35955299222762	-0.60635394138295
C	-3.80346684755035	-0.98663030760706	-0.29482298575796
C	-2.69062677393632	-1.40262088508754	0.43190923994013
C	-1.74897650753412	-0.47398512768286	0.84673581175998
O	-4.70007624054521	-1.93882065685839	-0.67246897950299
H	1.02454815991880	2.74444278592053	0.41211718743834
H	-0.49336341065563	1.66038112009836	1.97111666448193
H	-1.28794693047201	2.87976938689874	0.98108152233732
H	-3.13444092895075	2.32269206764135	-0.43180929490037
H	-4.81790654258386	0.69015402718748	-1.17224501383123
H	-2.58867197182992	-2.44961638364948	0.67744202467905
H	-0.89298618877089	-0.80209450885590	1.41865085898798

H	-5.43351603596270	-1.52598660474808	-1.13825335561139
H	-0.56439612480252	1.57718799623668	-1.75554612148922
C	2.55727115318010	-1.00645149202661	-0.98281004177998
C	3.95165112417344	-0.90935558035448	-0.36219898915025
O	3.98070760709932	-0.51726034436643	0.91046195949991
O	4.94484174435447	-1.19447257671991	-0.97296439880766
H	1.62098477791621	0.76663468470535	-1.76778935017252
H	2.67967816748882	-1.29859917792007	-2.01952700255662
H	2.00514978046493	-1.78484970412382	-0.45177726112399
H	3.06529882080362	-0.34818143102123	1.23552548955590
O	-1.36310145926431	-0.18251448720394	-2.64340973954583
H	-0.95468406161777	-0.99150910477894	-2.95974665419430
H	-1.98218008441460	-0.46016151959808	-1.95836201575268

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explicit-6_nh2-2.xyz

N	2.19234324858681	-0.88483136534606	0.42145904970388
O	1.29619253537295	-1.04387793571031	-1.64182186811495
H	-0.34563700324657	-2.89635192560594	2.00504264089165
C	-1.14639128781172	-2.07087333242730	-0.57325925017212
C	-1.82856791385512	-0.77068737430779	-0.25860135439425
C	-2.79134392727256	-0.69382881219517	0.74175925464405
C	-3.40131276786174	0.51194562785675	1.07123419890317
C	-3.05344132106962	1.67029730372806	0.38568575597661
C	-2.09209037359060	1.61357794128945	-0.61854092273254
C	-1.49220203228502	0.40558172960614	-0.93301122174619
O	-3.61769461068600	2.88207339578889	0.65233215723264
H	0.55828067789139	-3.26492645734217	-0.11098729473152
H	-0.97217978976063	-2.15687314391776	-1.64470092094168
H	-1.78982584364231	-2.89933017493679	-0.27292423227846
H	-3.07555282123032	-1.58933821014862	1.27784408241093
H	-4.15143281301022	0.54881550649245	1.85121908637945
H	-1.82785782554000	2.52050823830416	-1.14193165742049
H	-0.74060886327663	0.36925821967679	-1.70783531605615
H	-4.26676994218155	2.78568362599556	1.35536382946408
H	-0.17955015684744	-1.25487496940544	1.88943534757900
C	3.21654554825605	0.01002024590688	-0.01449043580094
C	2.72061749438417	1.42752914969485	-0.21134736561665
O	3.62523068829095	2.16082889719468	-0.87279636112012
O	1.67451263678335	1.87554731561057	0.18199827100119
H	2.05517091430180	-1.11989647330122	1.39178348426573
H	3.63562275738008	-0.32550423107423	-0.96144844422455
H	4.02234974232176	0.04060991986558	0.71780061288960
H	3.27142034005568	3.05868818362902	-0.95185932907651
O	-0.13509993355362	0.81114975022645	2.16873500468658
H	-1.02167018219872	1.05157799262433	1.88122143272302
H	0.44693795196841	1.17485669993971	1.48486106957298

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explicit-7_nh2-2.xyz

N	2.55150739101283	-0.03342388964737	0.74702867834226
O	2.02583535005463	1.78980619812172	-0.50313909161972
H	0.95614872833528	-1.77676611366846	-0.88363752780732
C	-0.61225560772670	0.69628106921529	0.72616652057782
C	-2.03653623253181	0.26677200690968	0.51570309831137
C	-2.74243126712410	0.66342245743760	-0.61810486294471
C	-4.05219776686230	0.25273874059768	-0.83361894924560
C	-4.68664297115098	-0.56212927672015	0.10079162268158
C	-3.99955534407382	-0.96595434813423	1.23898519588505
C	-2.68945949755815	-0.55267677172689	1.43367006498984

O	-5.96804768527172	-0.99615868908612	-0.05093409409489
H	0.06814802624845	0.40526499936834	-1.28749048782786
H	-0.28949409086307	0.41477438824081	1.72906530237375
H	-0.52869620463483	1.77997351010727	0.63911708238860
H	-2.26493587812723	1.30432328394563	-1.34724088724405
H	-4.58494267947161	0.57553892355391	-1.71920694199374
H	-4.50319980506184	-1.59227129484455	1.96081343197112
H	-2.16096509676769	-0.87489466015354	2.32038172614457
H	-6.34005488599185	-0.63105484653231	-0.85931285028977
H	-0.52168736810543	-1.77338782711120	-0.22285311466188
C	3.92967915262625	0.31738142555445	0.89354159367955
C	4.80394654677920	-0.33240860375764	-0.15849186502281
O	6.08597372307955	0.05094217835474	-0.01310385803526
O	4.43129600056297	-1.09623752454723	-1.00594295889379
H	2.24351929203240	-0.97632955592916	0.93199979447211
H	4.30568964524999	0.03084434758600	1.87530826039561
H	4.03249638737225	1.39677241927764	0.79939097531204
H	6.59726483524694	-0.38913186245164	-0.70721095300341
O	-2.27564823720721	-2.70108741537770	-1.14643256993392
H	-2.78585630234318	-3.16907931059371	-0.48042887571150
H	-2.72601774471856	-1.85294269504935	-1.23090622644998

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explicit-9_nh2-2.xyz

N	2.39386609369864	-0.53654582419464	1.40536049581933
O	1.96631712664624	-2.12296544339310	-0.16548185910361
H	-0.12232542420017	-0.87551487015733	2.83915536787296
C	-0.38280063267157	-0.21658273423110	-0.41624231744872
C	-1.85966071125718	0.05193157344637	-0.39710082436659
C	-2.36351589503225	1.29656251440387	-0.03506861446708
C	-3.73256514151785	1.53349550008151	0.01883651130664
C	-4.62224327037407	0.51440488563280	-0.29362593334635
C	-4.13806661081001	-0.73768414497595	-0.66041651545520
C	-2.77258787875215	-0.95758153134542	-0.70787867389036
O	-5.97435884002379	0.68072424666440	-0.26371754194426
H	-0.41869627469752	-1.99210810662400	0.79486602443694
H	0.17341181491628	0.72129486288710	-0.44381434054902
H	-0.10814197171019	-0.78987579435267	-1.30055585789340
H	-1.67691624538256	2.09808872925896	0.20236859481534
H	-4.10552734241031	2.51096723169475	0.29768512761054
H	-4.84134465379592	-1.51890638757489	-0.90846588125838
H	-2.40465356224753	-1.93258193226752	-0.99954190584109
H	-6.18005366410400	1.58491392579778	-0.00904217453312
H	-1.09819518377035	0.14789034926843	2.00336099516331
C	3.76776172728968	-0.39679103013012	1.01456196035625
C	3.93908603558601	0.56556668198037	-0.14329706582737
O	5.22397268987638	0.61342451680536	-0.53503111724633
O	3.06322220897373	1.21499002996994	-0.64477526030507
H	1.92470108143619	0.24021361430707	1.85412806452745
H	4.15827781373939	-1.36490949476725	0.70877254591432
H	4.36958287828509	-0.04137511466709	1.84975507273823
H	5.27857101735582	1.23911772566306	-1.27171231328479
O	1.35204513261661	-2.44592421550117	3.57925866991595
H	1.97051945937494	-1.93568160822256	3.04134639176431
H	1.42649063566210	-3.34802443964702	3.25848427965078

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explicit-11_nh2-2.xyz

N	-2.59228572564828	0.12709921433122	0.14423142012248
O	-1.79103021301657	2.23950123746956	0.08532790547907

H	-0.74104278439974	-0.82740212963717	2.07100168040031
C	0.57769259086084	0.47794545535573	-0.70557657809465
C	2.00856598432799	0.06629805481844	-0.50608910054583
C	2.89764862527989	0.88605890372497	0.18561626557177
C	4.21690467690554	0.50428190590721	0.39688432345513
C	4.67407069258450	-0.71465437297713	-0.09789976685876
C	3.80224935483020	-1.54503962978447	-0.79155050824887
C	2.48630715187359	-1.15103198254902	-0.98633151875764
O	5.95454709137782	-1.14469510475035	0.07279428086625
H	0.21766284964551	1.21771921494870	1.27433133973344
H	0.09515164076894	-0.20625012097388	-1.40483353198916
H	0.52733688044229	1.48140450230130	-1.12804700800160
H	2.55793907676604	1.83997722450233	0.56648571787402
H	4.89337920739953	1.15790689642478	0.93301420668210
H	4.16877686929379	-2.48543320221748	-1.17660244349507
H	1.81336141518830	-1.80497421586651	-1.52377917395259
H	6.46114597824585	-0.47490412402324	0.54173067682424
H	0.61103475372264	-1.24409620592799	1.29124889634470
C	-3.92070498723428	0.51775499830650	-0.22869752385850
C	-4.83274354413832	-0.67618487545674	-0.22363483071712
O	-6.08742707163642	-0.32403796615576	-0.54938359240711
O	-4.50509346957626	-1.80492213556863	0.02986533746327
H	-2.37034083807033	-0.84878382066886	0.27837449284370
H	-3.94675329664109	0.97243422046001	-1.22166855345387
H	-4.31702832806151	1.27055631554329	0.45454445485978
H	-6.62424402599624	-1.12935328328581	-0.53447904304302
O	2.47114374566633	-1.75761006631339	2.35274929642866
H	2.94900574598788	-1.03271933613833	1.93379986420611
H	2.84314522985887	-2.54575759544344	1.94862687595540
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explicit-16_nh2-2.xyz			
N	-2.72447511585592	-0.35030631968291	-0.55729459881709
O	-2.20561528220507	1.76079468579380	-1.18051111511492
H	-1.15055272085087	-0.14022349296241	1.86393665205433
C	0.47299592743650	0.11495743445915	-1.04067704167857
C	1.86714723489671	0.02749911017442	-0.48951201718346
C	2.44278041636326	-1.19791072673727	-0.17194980777686
C	3.71733354306818	-1.27504599061882	0.37775371949692
C	4.43742225683532	-0.11200226934101	0.61720274058518
C	3.87890688247505	1.12380144347257	0.30417256322306
C	2.60869270977865	1.18383585061402	-0.24134017302637
O	5.69042629262717	-0.11674932735643	1.14958771446061
H	-0.26992286028552	1.50473629553473	0.41462761767425
H	0.17329439551305	-0.84892555257086	-1.45427853962593
H	0.42439391971052	0.85489041417128	-1.83946578856819
H	1.89167477620484	-2.10947794586388	-0.36069080673442
H	4.15097656583378	-2.23859636489781	0.61351655152410
H	4.45289608964823	2.01968886000477	0.48907072200971
H	2.18437921531348	2.14879176474622	-0.48595517489526
H	5.96732021869500	-1.02308996364522	1.31312885477481
H	0.29769048869496	-0.75800306801910	1.38293340157189
C	-4.09367370020569	-0.28502015730805	-1.02673950748242
C	-4.94332431490240	0.58260459652356	-0.10141991468274
O	-4.63697331703528	1.88537170403682	-0.11484393922417
O	-5.79805301974871	0.14135729855805	0.61800977438904
H	-2.42781601106459	-1.09055432776668	0.06318789636638
H	-4.51262968772267	-1.28471459707264	-1.03781972394909
H	-4.10641178027912	0.12891029041184	-2.03473763661395

H	-3.83886267610238	2.03467480338540	-0.67841589427686
O	-3.12099216927929	0.96342221790287	2.38114018861306
H	-3.91411746477774	0.45919177491133	2.58775317660806
H	-3.46021446438662	1.73299733454010	1.91127975281265

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explicit-17_nh2-2.xyz

N	2.51418401712888	-0.26782375478927	-1.20271436138828
O	2.27780252648690	1.16557540040140	0.61253649207858
H	-0.74872225169865	-1.15040059488604	-1.55346615764402
C	-0.48131054218897	0.62474722772340	0.69012710897782
C	-1.93862904744979	0.32423708137672	0.47566481776538
C	-2.49655131230916	-0.86242800808375	0.94168225787597
C	-3.83044727478136	-1.17436061618000	0.70412627359385
C	-4.62983526476262	-0.29193845118227	-0.01175878895039
C	-4.08997457707715	0.90020849005401	-0.48598470436154
C	-2.75984170193014	1.19655668886005	-0.24138647403746
O	-5.94212004456473	-0.53374601548948	-0.27684285008874
H	0.01722247323784	1.05927482421571	-1.36630749812850
H	-0.07918835237225	0.00521184763907	1.490034111111615
H	-0.32123384846993	1.66018875013174	0.98277719714364
H	-1.88294714681774	-1.54769683369600	1.51207160686003
H	-4.24954188104013	-2.09733691016207	1.08436328266626
H	-4.72566504497724	1.58233986872892	-1.03087188073692
H	-2.35416152073134	2.13246949956884	-0.60336366730198
H	-6.20607042048484	-1.36608262597129	0.12639972928035
H	0.26553845312808	-1.66426342857666	-0.29691558672757
C	3.94877326292288	-0.36506135308457	-0.98648359189555
C	4.21166962885773	-1.31053408627571	0.17630544627899
O	3.67218236056941	-0.90619637608807	1.35171408397400
O	4.77528556348472	-2.36666009937036	0.09255799702127
H	1.00360280915247	-1.12846037921993	-1.67501234093661
H	4.38934526392624	0.61073144519242	-0.75609796020566
H	4.42840971303354	-0.78167711630107	-1.86587600817211
H	3.26947875263006	0.00248414346622	1.23562063688279
O	1.14482342732684	-2.31809631705196	1.20650760431689
H	1.31567883479235	-3.24646683011300	1.38456484258638
H	1.99790162628343	-1.87330085779515	1.36818551794463

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explicit-4b_nh2-2.xyz

N	0.88184121645593	2.19361004464754	0.86433101537391
O	0.89039303927608	1.71885998652545	-1.33930035620744
H	3.31758398618902	-0.32358383409441	1.72212733760610
C	2.20677122907093	-0.77225483645382	-0.83752095987319
C	1.00643339485571	-1.60614830900279	-0.49257859559693
C	1.12206818356384	-2.72126905534738	0.33487299796506
C	0.01564036140033	-3.47471500325164	0.70272705913598
C	-1.24310531056148	-3.11739526070491	0.23294708540060
C	-1.37979962577355	-2.00846024508041	-0.59548595298578
C	-0.26433748512631	-1.26559460264544	-0.95347040830136
O	-2.30201256524746	-3.88612242748042	0.61490242290786
H	3.32462872006824	0.94169619123328	-0.23272638953701
H	2.14030248293875	-0.41911015386117	-1.86539182467929
H	3.10860310550831	-1.38024776666677	-0.75135425207625
H	2.09810404494292	-3.01087458021485	0.70070508354967
H	0.11266511347110	-4.34143597085838	1.33993425219262
H	-2.35922048105525	-1.72397581871562	-0.95888314501130
H	-0.38089717539527	-0.39962394838364	-1.58819127378726
H	-3.10850448008281	-3.53185289252683	0.22897506507158

H	1.66791059769669	-0.31129404101152	1.83402931811356
C	-0.14809123107254	3.17221990677315	0.71936411669074
C	-1.52110819905549	2.56263485704207	0.52548781397060
O	-1.82500612329204	1.41467350259976	0.72622022964861
O	-2.39850076155115	3.48869332650129	0.11727626751587
H	1.24059454949405	1.91427401647214	1.76363548908782
H	0.05051981543992	3.81110270407857	-0.13943335300032
H	-0.18937545111124	3.80354607920425	1.60597650022742
H	-3.26095188205621	3.05697705392380	0.03334538266269
O	-0.35980016770480	-0.47562960453884	2.36992880931148
H	-0.85205621199252	0.10758507104360	1.77348007226857
H	-0.53920619599991	-1.36367367223028	2.04443386489847

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explicit-4c_nh2-2.xyz

N	-0.09161666228209	-1.66807787736569	-0.84971839900111
O	-0.00433727244178	-1.26507797663127	1.38188121601032
H	3.04961562742169	-0.04732353418531	-1.54448370756444
C	1.86333653428508	0.86276237661309	0.89627758952128
C	0.88958630215598	1.91913844148816	0.45703554168898
C	1.27160310354653	2.92978286124297	-0.42484454120232
C	0.37200040975765	3.88777907901324	-0.87084917223409
C	-0.94581068021888	3.85189952801148	-0.42720011135716
C	-1.34870617747777	2.85215145379435	0.45433541038161
C	-0.43633964614190	1.89971811224859	0.89062259179207
O	-1.79201883080155	4.81716641796344	-0.88331614885833
H	2.56283494269023	-1.10490667785610	0.43562860835014
H	1.67235680175741	0.58060233775036	1.93049592039122
H	2.88017361468644	1.25364001777676	0.83813592127660
H	2.29611112568665	2.97229290989635	-0.76999093003781
H	0.67576228112349	4.66952792054700	-1.55153480984058
H	-2.37239430439861	2.82464986849047	0.80696726341260
H	-0.75622609016275	1.12729732546908	1.57554652433657
H	-2.66414490386003	4.68808939054334	-0.49882472363109
H	1.50497484256449	0.47096400011449	-1.79431769251670
C	-1.14503234571673	-2.63345276478251	-0.71271316678068
C	-0.62655327513494	-4.00782580361813	-0.33821902268409
O	0.52871419541461	-4.32035909925580	-0.25511677955837
O	-1.64980249948978	-4.85577274845463	-0.12456590639633
H	0.53058114340168	-1.71853314384481	-1.64600614091879
H	-1.70328917580143	-2.71826800469625	-1.64420760434609
H	-1.83496065586039	-2.31062818682679	0.06398319340310
H	-1.26763663965276	-5.71498299256798	0.10517860408942
O	-0.61422564503148	0.94671164190419	-2.44398967432551
H	-0.75395393818647	1.77082465308411	-1.96535883640723
H	-0.79593005983770	0.25193577245879	-1.80094159788081

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explicit-1_oh.xyz

N	-1.50210800	-0.32279800	-0.89042700
O	-1.88074200	-0.81484100	1.28084200
H	-0.23449000	-3.51602900	-1.67978500
C	0.64807400	-2.32448500	0.96356200
C	1.49773800	-1.11478000	0.69711900
C	1.20018400	0.09013900	1.33161600
C	1.80486200	1.27618900	0.95639900
C	2.73599300	1.28757300	-0.08325100
C	3.11108900	0.07974300	-0.66892000
C	2.49509800	-1.10200400	-0.27907100

O	3.29427600	2.42971800	-0.53263400
H	-1.21118700	-3.19907400	0.29403700
H	0.26870600	-2.30480300	1.98374000
H	1.21225700	-3.24796500	0.82725700
H	0.46277100	0.10268300	2.12044000
H	1.54645100	2.20006900	1.45214100
H	3.86785500	0.08661600	-1.43984700
H	2.80024900	-2.03080500	-0.74611900
H	2.72789800	3.18152600	-0.26264500
H	0.75330500	-2.21487800	-1.56668600
C	-2.23493400	0.92653900	-0.88485800
C	-1.52598000	2.00692200	-0.07095500
O	-1.48185000	1.80032700	1.23256200
O	-1.05071900	2.99333300	-0.58446800
H	-1.09643900	-0.68521200	-1.74076300
H	-3.22876000	0.76577400	-0.46303200
H	-2.32688500	1.27999300	-1.90521700
H	-1.78390800	0.87590800	1.43347200
O	1.36180300	4.29449600	0.10655200
H	0.48923200	3.89563600	-0.06249300
H	1.33040100	5.17030400	-0.28344700

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explicit-2_oh.xyz

N	1.65156800	-0.00302000	-0.75914800
O	1.52861000	0.38574400	1.46031600
H	0.04528700	3.00267400	-1.71249700
C	-0.83009100	1.96291800	0.92455600
C	-1.82302400	0.88884500	0.57988900
C	-1.66228400	-0.41696400	1.04407100
C	-2.54417600	-1.42405300	0.68176400
C	-3.61864000	-1.14305500	-0.16266700
C	-3.79799800	0.15575800	-0.62864000
C	-2.90784400	1.15227600	-0.25627100
O	-4.51051900	-2.08416700	-0.54803600
H	1.04724600	2.77790600	0.27365300
H	-0.48557100	1.85495500	1.95135000
H	-1.29556100	2.94422400	0.82670300
H	-0.83599300	-0.64448000	1.70331900
H	-2.41131300	-2.43031800	1.05462200
H	-4.64111900	0.36901800	-1.26936200
H	-3.07067800	2.16229300	-0.61073500
H	-4.29190500	-2.94056500	-0.14266300
H	-0.78076700	1.59417600	-1.62769900
C	2.35137400	-1.26723700	-0.64295700
C	3.80998100	-1.14168200	-0.20173700
O	4.00104700	-0.51428400	0.95730500
O	4.71436200	-1.60283900	-0.84298800
H	1.41382000	0.38484300	-1.66029800
H	2.34003800	-1.76100400	-1.60772200
H	1.82892100	-1.89060700	0.08560300
H	3.13610900	-0.22420300	1.33383200
O	-3.92816500	-4.55599100	0.63081000
H	-4.55104800	-4.86212800	1.29516000
H	-3.76845000	-5.30317200	0.04855200

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explicit-3_oh.xyz

N	-2.00936600	-0.61406100	-0.78274400
O	-1.93458700	-1.04986000	1.43122000

H	0.01301300	-3.34783600	-1.71425800
C	0.71476800	-2.14050200	0.93819100
C	1.54250300	-0.94786400	0.54902200
C	2.69902500	-1.09675900	-0.21203500
C	3.44025400	0.00087500	-0.63317200
C	3.02528800	1.28645000	-0.29403400
C	1.87173500	1.45334700	0.47053000
C	1.14687200	0.34986300	0.88466400
O	3.70124100	2.39547200	-0.67091900
H	-0.98135700	-3.28193400	0.27858400
H	0.33890500	-2.04001000	1.95494800
H	1.32518500	-3.04304800	0.89290900
H	3.03956300	-2.09157700	-0.47087100
H	4.34049500	-0.13348900	-1.21702000
H	1.55730000	2.45273800	0.73319700
H	0.26066600	0.50150700	1.48389100
H	4.48798700	2.15011800	-1.18650500
H	0.68034200	-1.85892700	-1.59890100
C	-3.09742000	0.34198400	-0.70566800
C	-2.70965500	1.67286000	-0.05909100
O	-2.24942200	1.58301500	1.18865800
O	-2.84031200	2.72338600	-0.62454600
H	-1.63347400	-0.90539800	-1.67323900
H	-3.91456400	-0.09203000	-0.12534300
H	-3.44492100	0.55351900	-1.71014800
H	-2.22057400	0.63640000	1.46947000
O	6.01349200	1.77495300	-2.13083600
H	6.82340600	2.01929700	-1.67512200
H	6.06119800	2.18796100	-2.99710800

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explicit-4_oh.xyz

N	1.93926900	-0.48632800	0.03605500
O	1.14878300	-1.42418200	-1.85694100
H	0.07646600	-2.59880000	2.23576300
C	-1.16388600	-2.28850600	-0.38039000
C	-1.90919500	-0.99039100	-0.24770300
C	-1.70833800	0.05260400	-1.15221400
C	-2.35749700	1.26950100	-1.00378100
C	-3.23066700	1.47151600	0.06468000
C	-3.44545700	0.44104800	0.97397300
C	-2.78955600	-0.77054700	0.81139100
O	-3.89297400	2.63771400	0.25689000
H	0.69106000	-3.22059100	0.15887600
H	-1.06302500	-2.56772300	-1.42758600
H	-1.71254500	-3.08168500	0.12968700
H	-1.03278400	-0.09529800	-1.98313900
H	-2.19589000	2.06758200	-1.71549300
H	-4.13231300	0.60042300	1.79241200
H	-2.97809300	-1.56950800	1.51725100
H	-3.67890000	3.26373900	-0.45471900
H	-0.38702400	-1.09354500	1.80821700
C	2.84482800	0.37581400	-0.66362100
C	3.61370800	1.22240300	0.31025900
O	4.44623600	2.05919300	-0.33324600
O	3.51894400	1.17474600	1.50764800
H	1.92576100	-0.50430900	1.04534800
H	2.31350100	1.02942500	-1.35779000
H	3.55433100	-0.19115700	-1.27050900

H	4.91601900	2.56880900	0.34230800
O	-3.32716500	4.47631900	-1.78993800
H	-4.05161200	4.65829000	-2.39408300
H	-2.98346700	5.33132700	-1.51866700

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explicit-5_oh.xyz

N	1.70941900	0.03692900	-0.77190600
O	1.55348000	0.37328200	1.45424300
H	0.07741600	3.04386700	-1.67520700
C	-0.82135800	1.92979600	0.92469800
C	-1.80070900	0.85816500	0.53668000
C	-2.88240900	1.13904000	-0.29384600
C	-3.76330300	0.14584300	-0.70539000
C	-3.57110500	-1.16662400	-0.28147000
C	-2.49745000	-1.46370300	0.55657000
C	-1.62815400	-0.46360100	0.95661600
O	-4.39080200	-2.18080000	-0.64128700
H	1.05321800	2.78343600	0.31832200
H	-0.48893400	1.79522700	1.95237800
H	-1.29431000	2.90951500	0.84899400
H	-3.05376200	2.15873100	-0.61525600
H	-4.60187200	0.38314700	-1.34519400
H	-2.36640000	-2.48263400	0.89086800
H	-0.80310300	-0.70463900	1.61254200
H	-5.11388200	-1.84804900	-1.19946100
H	-0.73772400	1.62669400	-1.63273900
C	2.43499200	-1.21460300	-0.67543600
C	3.88650600	-1.06321300	-0.21955000
O	4.05219600	-0.46249400	0.95775500
O	4.80800700	-1.48071800	-0.86613300
H	1.47785200	0.44198300	-1.66694500
H	2.44237000	-1.68864900	-1.65006400
H	1.92024000	-1.86398000	0.03549700
H	3.17752900	-0.20399800	1.33392400
O	-6.47085100	-1.24468900	-2.27270700
H	-6.52975800	-1.65599600	-3.13905300
H	-7.35404200	-1.28767300	-1.89668900

31

explicit-6_oh.xyz

N	1.86752800	-0.42168100	0.08262800
O	1.11815900	-1.40380200	-1.80478400
H	-0.02021100	-2.51160200	2.28733100
C	-1.22288000	-2.23207100	-0.34976400
C	-1.96329900	-0.92854900	-0.24730200
C	-2.85623500	-0.68824300	0.79357800
C	-3.50756400	0.53214100	0.92993800
C	-3.27065300	1.54748100	0.00741700
C	-2.38478300	1.32206200	-1.04419900
C	-1.74220100	0.10164100	-1.16551300
O	-3.87339100	2.75875300	0.07991000
H	0.62151400	-3.16280100	0.22849300
H	-1.10828700	-2.52755600	-1.39107000
H	-1.78196700	-3.01504800	0.16480200
H	-3.06075100	-1.47519700	1.50854400
H	-4.20208000	0.69880300	1.74173500
H	-2.21692200	2.11331100	-1.76052400
H	-1.05644300	-0.06397800	-1.98455800
H	-4.47529900	2.78720700	0.84196700

H	-0.47627400	-1.01193700	1.83237800
C	2.77613500	0.43681400	-0.61802000
C	3.51188000	1.31625700	0.35243300
O	4.34898400	2.14724100	-0.29154900
O	3.38925000	1.29592800	1.54832900
H	1.83690600	-0.41829500	1.09153400
H	2.25030500	1.06690200	-1.33759600
H	3.50614400	-0.13343500	-1.19679800
H	4.79417700	2.68197000	0.38121000
O	-5.60191200	2.89216600	2.29433400
H	-6.53634000	2.99599000	2.09647500
H	-5.38629200	3.57606200	2.93367700

31

explicit-7_oh.xyz

N	2.42463800	-0.16022400	0.64908100
O	1.97756300	1.91258000	-0.16917200
H	0.63994300	-1.46886100	-1.34746600
C	-0.72838400	0.70480800	0.77290100
C	-2.15462700	0.37502300	0.43718700
C	-2.86789300	1.14656400	-0.47807900
C	-4.17012700	0.82908300	-0.83265500
C	-4.79266100	-0.28554200	-0.26998200
C	-4.09567700	-1.06630900	0.64631100
C	-2.79365200	-0.73301300	0.99083500
O	-6.06201400	-0.64429500	-0.57600900
H	-0.02062600	0.79412100	-1.24765100
H	-0.43942300	0.21178900	1.70247100
H	-0.60364800	1.77856000	0.90930400
H	-2.39749800	2.01620300	-0.91885600
H	-4.71264500	1.44060200	-1.54042500
H	-4.58784600	-1.92302000	1.08314000
H	-2.26413500	-1.34313900	1.71111300
H	-6.44515200	-0.01291900	-1.20756000
H	-0.73725800	-1.51806200	-0.47064200
C	3.81140600	0.09818400	0.87875300
C	4.68405400	-0.37739500	-0.26337100
O	5.97684400	-0.08672000	-0.02578500
O	4.30315300	-0.94857500	-1.24805100
H	2.08002000	-1.10796000	0.61817800
H	4.15617200	-0.38240200	1.79419800
H	3.95592600	1.17117700	0.99133600
H	6.48638500	-0.40915600	-0.78281100
O	-7.22933900	1.17988200	-2.36011100
H	-7.56323400	0.83178800	-3.19086800
H	-7.93745100	1.71251400	-1.98896400

31

explicit-9_oh.xyz

N	2.61790100	-0.50597800	0.96925200
O	2.14417000	-1.90337500	-0.75602500
H	0.19665700	-1.15554700	2.53455900
C	-0.29180000	-0.10170000	-0.58435000
C	-1.77376100	0.08333900	-0.42924300
C	-2.30502600	1.24222500	0.12811600
C	-3.67425700	1.39938500	0.31124400
C	-4.54461600	0.38177100	-0.06905700
C	-4.02900300	-0.78532400	-0.63054800
C	-2.66312300	-0.92545400	-0.80385000
O	-5.88809400	0.47296300	0.07822400

H	-0.16222300	-2.01878500	0.37201500
H	0.21921700	0.86020800	-0.51966900
H	-0.05497400	-0.53738100	-1.55385800
H	-1.63725900	2.04295400	0.41845800
H	-4.07140800	2.30823200	0.74195300
H	-4.71395600	-1.56526900	-0.92985600
H	-2.27666100	-1.83427600	-1.24702700
H	-6.12483800	1.34013700	0.44743900
H	-0.85086800	-0.08611500	1.88577800
C	3.98338000	-0.33128500	0.58226700
C	4.16491100	0.79657500	-0.41307900
O	5.44846200	0.87324900	-0.81292400
O	3.30526600	1.54099600	-0.79584600
H	2.17334200	0.15013400	1.59350700
H	4.34578000	-1.24745600	0.12043300
H	4.60842300	-0.12472300	1.45025700
H	5.50776900	1.60428400	-1.44447200
O	-6.63330200	2.98874000	1.07766400
H	-7.18793100	3.00320800	1.86188000
H	-7.06982200	3.54960200	0.43115700

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explicit-11_oh.xyz

N	-2.54118600	0.13120300	0.15947800
O	-1.83533900	2.27276000	0.00424200
H	-0.47244800	-0.68015400	2.11845400
C	0.61569500	0.60117800	-0.75342300
C	2.06433700	0.27825500	-0.52429700
C	2.93699700	1.24114400	-0.02130800
C	4.26741700	0.94802000	0.23680900
C	4.75705500	-0.33558100	-0.00619200
C	3.90002700	-1.30886000	-0.50931700
C	2.57196800	-0.99760700	-0.76335300
O	6.04637000	-0.68024800	0.22402700
H	0.23556700	1.37864800	1.20500500
H	0.17033700	-0.13597500	-1.42400800
H	0.50774600	1.58277100	-1.21292300
H	2.57041400	2.24215600	0.16690200
H	4.93388900	1.70777000	0.62132900
H	4.28906600	-2.29800700	-0.70212200
H	1.91696700	-1.76078100	-1.16338400
H	6.54388500	0.08718300	0.55268700
H	0.72667800	-1.12059300	1.10516600
C	-3.89382800	0.44890100	-0.19291700
C	-4.76890600	-0.76290100	-0.04234900
O	-6.04466700	-0.47625600	-0.35171400
O	-4.39983000	-1.85435500	0.30152300
H	-2.27601100	-0.82372500	0.35166500
H	-3.97444000	0.80940500	-1.22122400
H	-4.28425600	1.25100100	0.43534200
H	-6.55538200	-1.29125600	-0.24311800
O	7.54577200	1.52402000	1.10033100
H	8.00659000	1.44738900	1.93973300
H	8.19720100	1.83107000	0.46440600

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explicit-16_oh.xyz

N	-2.46719900	-0.76487400	-0.11392200
O	-2.12650500	1.43811600	-0.48485800
H	-0.40240500	-0.95854200	2.06783300

C	0.62077400	0.15121600	-0.89188800
C	2.07906000	0.09122600	-0.53964200
C	2.80025100	-1.09424300	-0.64050600
C	4.13943300	-1.16275500	-0.27445600
C	4.78487400	-0.02604400	0.20523900
C	4.07599800	1.17052300	0.30952000
C	2.74344000	1.22068400	-0.05833300
O	6.08561900	-0.02275100	0.57514500
H	-0.03492400	1.05589900	0.93805200
H	0.34829400	-0.71295100	-1.50063600
H	0.39674000	1.04941000	-1.46591500
H	2.31175400	-1.98163800	-1.02223800
H	4.68797200	-2.09007700	-0.36439500
H	4.58899200	2.04839200	0.67422700
H	2.20778800	2.15788000	0.02193000
H	6.47365300	-0.90530400	0.44741300
H	0.86093100	-1.34827800	1.11473600
C	-3.79495100	-0.80450600	-0.69784700
C	-4.86553200	-0.11807500	0.15056500
O	-4.63799300	1.16621100	0.42080100
O	-5.85209200	-0.69110600	0.52454000
H	-2.02935000	-1.60138500	0.24247800
H	-4.08848900	-1.84010300	-0.82467800
H	-3.76823500	-0.31510200	-1.67357700
H	-3.78234400	1.45266500	0.02226900
O	7.24219300	-2.55004600	0.23566300
H	7.96242400	-2.59659800	-0.39870100
H	7.57167900	-2.95297600	1.04330400

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explicit-17_oh.xyz

N	2.64188200	-0.48854300	-0.90968300
O	2.11487100	1.52758900	-0.04385000
H	-0.75414600	-1.55423500	-1.29325600
C	-0.48373600	0.54903300	0.62798200
C	-1.95926100	0.32436500	0.47200700
C	-2.60244000	-0.74596500	1.08429400
C	-3.95901700	-0.98275500	0.89838200
C	-4.70380300	-0.13679700	0.08039800
C	-4.07542400	0.94163300	-0.53990600
C	-2.72313700	1.16207300	-0.34194400
O	-6.02758600	-0.30983400	-0.14086900
H	-0.07131300	0.58633000	-1.47422800
H	-0.11327700	0.02185600	1.51068900
H	-0.25795900	1.60452900	0.76805700
H	-2.03828200	-1.40427300	1.73249000
H	-4.44496900	-1.81598700	1.38682800
H	-4.66374900	1.59844900	-1.16384300
H	-2.25128300	2.00999100	-0.82226000
H	-6.35575300	-1.07078100	0.36751300
H	0.16273000	-1.90074900	-0.00386900
C	4.06306900	-0.21927300	-1.02596400
C	4.79873600	-0.19748600	0.31373200
O	4.34287100	0.68977300	1.19702400
O	5.73512300	-0.91285700	0.54329200
H	2.24479500	-1.34695900	-1.26108000
H	4.20377100	0.75034700	-1.50817900
H	4.51436200	-0.99223700	-1.63708900
H	3.58037700	1.18643600	0.81755900

O	-7.02384400	-2.48213500	1.32237000
H	-7.60821300	-2.25465500	2.05036000
H	-7.47697200	-3.16346600	0.81899500

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explicit-4b_oh.xyz

N	0.40627300	1.82893600	0.67617100
O	1.13332400	1.76181200	-1.47036800
H	3.07239800	-0.12524600	1.96252900
C	2.31985900	-0.80802200	-0.81182500
C	1.07146000	-1.62595900	-0.65177000
C	1.01363500	-2.70060500	0.23565400
C	-0.18560100	-3.33584900	0.52910100
C	-1.36351100	-2.90116100	-0.06990900
C	-1.30549000	-1.88250900	-1.02013800
C	-0.10641200	-1.24955700	-1.29575500
O	-2.53104000	-3.48943800	0.28588400
H	3.24683600	0.95312100	0.00833600
H	2.41716300	-0.43946100	-1.83134200
H	3.20164500	-1.40641800	-0.57890400
H	1.92179400	-3.03966100	0.71825300
H	-0.22969600	-4.14986500	1.23792400
H	-2.21145300	-1.57468300	-1.52017300
H	-0.08211300	-0.43431800	-2.00482600
H	-3.25050100	-2.84481200	0.15857700
H	1.59387500	-0.75114200	1.66050400
C	-0.65364100	2.74899500	0.42522400
C	-2.02863000	2.11924700	0.41889100
O	-2.28073400	0.94945300	0.55117000
O	-2.96787300	3.06279100	0.24439700
H	0.59798200	1.47039200	1.59890000
H	-0.49594600	3.19605400	-0.55686300
H	-0.66392000	3.55880500	1.15552000
H	-3.83335800	2.63075300	0.25886300
O	-4.19975800	-1.24159200	0.24121000
H	-3.55937400	-0.52850000	0.38603300
H	-4.74750600	-0.95992400	-0.49440300

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explicit-4c_oh.xyz

N	-0.19446900	-1.64833200	-0.60929500
O	0.14665900	-1.30086100	1.60306900
H	2.81960000	-0.05073900	-1.64219700
C	1.84659400	0.91973100	0.92556300
C	0.82689600	1.95050800	0.53098300
C	1.14595700	2.97560900	-0.35917400
C	0.20045600	3.90404400	-0.77013300
C	-1.10227400	3.82394600	-0.28916600
C	-1.43963200	2.80850900	0.60520800
C	-0.48338100	1.88698200	1.00559500
O	-1.99473300	4.75166800	-0.71193600
H	2.56965900	-1.02338200	0.37142300
H	1.72309600	0.63760200	1.96954000
H	2.85044600	1.32905000	0.80312000
H	2.16047300	3.05952000	-0.72784000
H	0.45752500	4.70073800	-1.45296700
H	-2.45045100	2.74948200	0.98503300
H	-0.75385100	1.10218000	1.69810200
H	-2.85470900	4.60567400	-0.28377800
H	1.36690100	0.69442700	-1.62888200

C	-1.26786700	-2.56811100	-0.40011800
C	-0.79446200	-3.99772800	-0.23668900
O	0.33447800	-4.38445700	-0.35381100
O	-1.83376400	-4.80787700	0.04635200
H	0.27321400	-1.58416600	-1.50057900
H	-1.96955600	-2.53574800	-1.23291800
H	-1.80799600	-2.28955800	0.50261700
H	-1.47908000	-5.70364900	0.13831500
O	-4.47689800	4.42044700	0.56016600
H	-4.67681100	5.09185700	1.21756100
H	-5.26080600	4.34191100	0.01064500

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explicit-1_ohcarbh.xyz

N	-1.88121200	-0.69538500	-0.56041900
O	-1.88399100	-1.44286000	1.58958100
H	-0.10111200	-3.45620700	-1.77511900
C	0.81912700	-2.31524700	0.91955200
C	1.51689100	-1.03396700	0.55814900
C	1.00184400	0.19716900	0.96413900
C	1.54302700	1.38920700	0.51439400
C	2.63392600	1.37183100	-0.34867900
C	3.19078500	0.15872400	-0.73371100
C	2.62745400	-1.02778700	-0.28461200
O	3.19606100	2.50977100	-0.83710500
H	-0.86746600	-3.50625500	0.30854300
H	0.50131200	-2.31042900	1.96064900
H	1.48962700	-3.16235600	0.77302300
H	0.15326200	0.22819000	1.63217900
H	1.09556500	2.32813000	0.81201000
H	4.04858300	0.15873100	-1.38991100
H	3.06330500	-1.96862600	-0.59590700
H	2.65445800	3.26423300	-0.58534300
H	0.71603900	-2.04542900	-1.59022100
C	-2.73006800	0.46135100	-0.37575300
C	-1.86695700	1.72210000	-0.24340200
O	-1.72971500	2.24402200	0.97053700
O	-1.31452700	2.19164400	-1.20342300
H	-1.45283100	-0.87114100	-1.45880400
H	-3.37159400	0.29863100	0.48410600
H	-3.34732300	0.58818700	-1.26124200
H	-2.20601700	1.72658200	1.66909200
O	-2.88759100	0.70301200	2.80464600
H	-2.56879100	-0.17075800	2.48083700
H	-2.64190200	0.77303600	3.72919700

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explicit-4_ohcarbh.xyz

N	1.98803300	-0.33435100	-0.10011400
O	1.08979900	-1.34955500	-1.90387900
H	0.27589000	-2.37980900	2.29000600
C	-1.08935600	-2.23614700	-0.26556400
C	-1.87107700	-0.95716800	-0.16085000
C	-1.75719000	0.03730900	-1.13203000
C	-2.44267900	1.23737700	-1.01066600
C	-3.25864200	1.46708100	0.09204000
C	-3.38911100	0.48827800	1.06841300
C	-2.69918000	-0.70770200	0.93343900
O	-3.95592600	2.62584200	0.26158600

H	0.82189300	-3.07893400	0.21304800
H	-1.03394700	-2.56621600	-1.30108400
H	-1.58382300	-3.01761300	0.31305400
H	-1.12244300	-0.13399000	-1.98965300
H	-2.34740200	1.99605000	-1.77761300
H	-4.03460700	0.67199000	1.91458900
H	-2.81918900	-1.47122200	1.69105200
H	-3.78592300	3.21177700	-0.48173100
H	-0.21999800	-0.89779600	1.81936700
C	2.83721400	0.51586900	-0.88245400
C	3.67761000	1.38614100	0.00971900
O	4.45912800	2.19542500	-0.68866000
O	3.64021700	1.34524000	1.22291800
H	2.04263100	-0.31660700	0.90758100
H	2.25494800	1.15683700	-1.54682900
H	3.49846200	-0.06355700	-1.52997700
H	4.98859500	2.74219900	-0.05830300
O	5.51230500	3.38137100	1.48432700
H	4.93385000	2.72351500	1.90244100
H	6.38422600	3.27562300	1.87107300

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explicit-6_ohcarbh.xyz

N	2.05641000	-0.49554500	-0.07409400
O	1.12963200	-1.44658200	-1.89885900
H	0.22689800	-2.48809000	2.27206500
C	-1.11586200	-2.21985200	-0.29087900
C	-1.82209100	-0.89928000	-0.16844900
C	-2.64853800	-0.62524600	0.91719700
C	-3.26775600	0.61098000	1.06399500
C	-3.06406700	1.59997700	0.11099200
C	-2.24614200	1.34480500	-0.98489000
C	-1.63473500	0.10965500	-1.11772700
O	-3.64215600	2.83187400	0.19232300
H	0.73831000	-3.18184300	0.18744600
H	-1.07125300	-2.53378100	-1.33194300
H	-1.65972700	-2.98145300	0.26966800
H	-2.82689800	-1.39411100	1.65761700
H	-3.91325100	0.80047300	1.91240600
H	-2.10531600	2.11993500	-1.72387200
H	-0.99936000	-0.08454700	-1.97003600
H	-4.18970200	2.87642000	0.98147500
H	-0.19521000	-0.97596900	1.82414300
C	2.94980300	0.32801700	-0.83539400
C	3.72146100	1.24567600	0.07129000
O	4.53227200	2.04099200	-0.60914100
O	3.61359600	1.24704900	1.28112600
H	2.09387000	-0.48558100	0.93435800
H	2.40397100	0.92754200	-1.56524400
H	3.66221300	-0.26798000	-1.41042600
H	5.01904400	2.61530600	0.03107000
O	5.53821000	3.22520900	1.58772100
H	5.36612900	4.10567100	1.92857700
H	4.88143500	2.63202900	1.98661000

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explicit-7_ohcarbh.xyz

N	2.58461500	-0.16348500	0.83170500
O	2.17356700	1.86298300	-0.10716200
H	0.89998100	-1.56213200	-1.18281000

C	-0.56803000	0.69077600	0.78517600
C	-1.98080100	0.35637100	0.40079700
C	-2.65095300	1.10568200	-0.56344400
C	-3.94006900	0.78124900	-0.95868800
C	-4.58567300	-0.31225100	-0.38998700
C	-3.93593100	-1.07168300	0.57422000
C	-2.64706600	-0.73277700	0.96011100
O	-5.85116400	-0.67931300	-0.73611600
H	0.21905700	0.70156600	-1.20784500
H	-0.32132600	0.22933000	1.74241100
H	-0.44469200	1.76821800	0.88923100
H	-2.15984900	1.96063900	-1.00920600
H	-4.44766400	1.37970900	-1.70473700
H	-4.45004700	-1.91325800	1.01442100
H	-2.15010800	-1.32382400	1.71800300
H	-6.19059900	-0.07274900	-1.40063300
H	-0.52566900	-1.58175800	-0.38725200
C	3.96229300	0.11587200	1.09590400
C	4.86590100	-0.23714800	-0.06788500
O	6.12677600	0.08999600	0.18103300
O	4.48002900	-0.76310700	-1.08994100
H	2.24814300	-1.11407700	0.83075300
H	4.30635800	-0.43229200	1.97199500
H	4.08194400	1.17800100	1.29961900
H	6.67531700	-0.15092500	-0.60433400
O	7.01543200	-0.80377700	-2.20481000
H	6.05858400	-0.96322600	-2.26337200
H	7.25120200	-0.25165900	-2.95374500

31

explicit-9_ohcarbh.xyz

N	2.66250948750787	-0.48960526802743	0.94494674985309
O	2.16772593903734	-1.91666329316581	-0.75087961081919
H	0.25285627087323	-1.07335386106304	2.52003273971255
C	-0.23377880612201	-0.07118118387711	-0.61933112539135
C	-1.71484999898262	0.13318841865390	-0.48207088960257
C	-2.23714385472007	1.30275402803058	0.05994589488443
C	-3.60748268976414	1.47481016091308	0.22272701024617
C	-4.48007008682282	0.46536664885453	-0.16092915984724
C	-3.97770358887208	-0.71189207688918	-0.70726442856800
C	-2.61128611978638	-0.86790029941119	-0.86138084607167
O	-5.83256598486209	0.57072153262358	-0.03190560270713
H	-0.13825541669045	-1.97441549969151	0.36882824989277
H	0.28836953668381	0.88505730789103	-0.56394121281817
H	0.00495871363205	-0.52396226920992	-1.58042481780297
H	-1.56466650687961	2.09747617295507	0.35419611151002
H	-3.99483389771515	2.39518363248753	0.64132250253224
H	-4.66841489431997	-1.48543701279924	-1.00893776677758
H	-2.22950673469584	-1.78401122352702	-1.29265062635943
H	-6.05255919610300	1.42890419377919	0.34205018202906
H	-0.81353926115943	-0.03017211526349	1.85990677972087
C	4.03041899063051	-0.33541629070202	0.55329722202920
C	4.22570352259918	0.75667108236568	-0.47962956304365
O	5.49633573430526	0.83787723967058	-0.85498251367286
O	3.33519643768302	1.46536811345091	-0.89292967897495
H	2.22742657666364	0.18791166379068	1.55233910725296
H	4.38821137235905	-1.26796252786502	0.12177217725695
H	4.65452021883915	-0.10595894191723	1.41576925114498
H	5.59112958096823	1.54982141909250	-1.52540664636894

O	5.00511852071806	2.84437371220283	-2.57525976909997
H	5.02169968663894	3.55157270579968	-3.22042444508078
H	4.09794748484759	2.72058134804084	-2.25985737133491

31

explicit-11_ohcarbh.xyz

N	-2.66415800	0.23340800	0.06209700
O	-1.84975800	2.34076500	-0.02981900
H	-0.70150500	-0.71795300	2.04935000
C	0.53434000	0.57272100	-0.75993100
C	1.96273100	0.18831600	-0.50070700
C	2.85767100	1.10758700	0.04197500
C	4.16866600	0.75448000	0.32461000
C	4.60947100	-0.53990600	0.06720900
C	3.73388500	-1.47139500	-0.47509100
C	2.42588900	-1.10181300	-0.75379600
O	5.88514900	-0.94527400	0.32185400
H	0.13811300	1.32584000	1.20488000
H	0.07817000	-0.13339400	-1.45577700
H	0.47872800	1.56611900	-1.20279200
H	2.52662900	2.11829600	0.24127700
H	4.85197300	1.48475300	0.73961500
H	4.08959400	-2.47066400	-0.67826300
H	1.75164400	-1.83019200	-1.18463200
H	6.38919300	-0.20984000	0.68210000
H	0.52234300	-1.18627400	1.07957200
C	-3.99128900	0.61820800	-0.32280900
C	-4.92478300	-0.55748000	-0.24520900
O	-6.16244800	-0.22517400	-0.57719900
O	-4.57677300	-1.67547000	0.07832300
H	-2.45041500	-0.73822100	0.23198100
H	-4.02114600	1.01520900	-1.34006200
H	-4.37043900	1.41456600	0.31922000
H	-6.73088900	-1.03160600	-0.51962100
O	-7.12201500	-2.72318300	-0.30466500
H	-6.19990400	-2.85757600	-0.03325800
H	-7.67617500	-3.08971300	0.38780000

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explicit-16_ohcarbh.xyz

N	-2.41296579274815	-0.36022973252384	-0.23829120761364
O	-1.85688281616675	1.83031689854585	-0.53206766851676
H	-0.46332159799913	-0.78628772708735	1.98194938281800
C	0.74898499698027	0.29834323220153	-0.92030948908259
C	2.19122550566363	0.12518558674895	-0.53975717534490
C	2.82343037193001	-1.10918200794462	-0.64246614210361
C	4.14717745180274	-1.27688444432864	-0.25156974000450
C	4.86008701860438	-0.19675428097331	0.25158378512337
C	4.24542999369834	1.04774038859882	0.35918310418933
C	2.92723967460492	1.19785929985328	-0.03288936740684
O	6.15817854559846	-0.29029624540699	0.64972638162638
H	0.13096642616471	1.22224593545806	0.91271523166468
H	0.42534684577068	-0.53481510603767	-1.54630623556614
H	0.60838087792287	1.21820781153718	-1.48625797331244
H	2.27924311132354	-1.95454362221616	-1.04234675848173
H	4.62353781143825	-2.24460243320510	-0.34425953196650
H	4.81461269565905	1.88087261852167	0.74415935128368
H	2.45976671969230	2.17043743853937	0.04872184129556
H	6.47239966327922	-1.18954667931215	0.51698132489431
H	0.81651382983820	-1.24556481077684	1.08085009096181

C	-3.79445601907351	-0.27586563046067	-0.66173718395553
C	-4.71293896370508	-0.23410386188827	0.56289058651872
O	-5.30976976724499	0.91693752530548	0.83852130068202
O	-4.85388289273549	-1.21418651421276	1.24702166692201
H	-2.05913009903869	-1.22432925815493	0.14810083090367
H	-4.04504130911007	-1.17658027175618	-1.21691394087620
H	-3.91168351088965	0.58431059504509	-1.31192488894621
H	-5.02105749736249	1.64794697989499	0.23638040659369
O	-4.33012963583753	2.86420594764371	-0.70513441690621
H	-4.39230197813070	3.76876991922869	-0.39208078317423
H	-3.37869714221507	2.61783322609220	-0.69394429698339

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explicit-4b_ohcarbh.xyz

N	-0.24180400	1.92200200	-1.06506600
O	-1.51951600	0.51252100	-2.30580500
H	2.83442500	0.50218100	-2.19212400
C	0.57462100	-1.41158000	-1.78675000
C	0.41000300	-1.53432400	-0.29742000
C	1.49097400	-1.84141400	0.52804000
C	1.38273700	-1.80685400	1.91195000
C	0.17296700	-1.45952800	2.49975400
C	-0.93391800	-1.20943700	1.69203000
C	-0.81152200	-1.24330800	0.31248800
O	0.10854600	-1.38873500	3.85626500
H	0.93549100	0.08901900	-3.29172400
H	-0.31775200	-1.75766400	-2.30445200
H	1.42140700	-2.01045000	-2.12417900
H	2.44018400	-2.10872800	0.08115300
H	2.22919100	-2.02763700	2.54564500
H	-1.88668000	-0.98051200	2.14994900
H	-1.67250000	-1.02918900	-0.30499000
H	-0.60781200	-0.78360700	4.09763200
H	2.21255000	0.23381800	-0.70308800
C	-1.34188200	2.52361400	-0.36681800
C	-1.27385400	2.20106500	1.11009700
O	-0.22955200	2.09714400	1.71931200
O	-2.47377200	2.06487100	1.66449300
H	0.70353800	2.08122200	-0.75135900
H	-2.26852500	2.14957100	-0.79177900
H	-1.33480500	3.61171900	-0.46491200
H	-2.35847800	1.82780800	2.60872200
O	-1.30056500	1.13909200	4.03556400
H	-0.59839600	1.45238900	3.43073100
H	-1.17649500	1.60345000	4.86777400

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explicit-4c_ohcarbh.xyz

N	-0.27900000	-1.75144100	-0.81141300
O	0.06136900	-1.53692000	1.41649500
H	2.77991700	-0.15625400	-1.74242100
C	1.85542600	0.64015300	0.89098400
C	0.86781700	1.73155200	0.58903700
C	1.21160500	2.80690900	-0.22997100
C	0.29616700	3.79699500	-0.55622900
C	-0.99757300	3.72355600	-0.05695600
C	-1.36055700	2.66277800	0.76613800
C	-0.43539100	1.67874600	1.08275900
O	-1.86461400	4.71792600	-0.39939200
H	2.49935500	-1.28214000	0.19241400

H	1.73281400	0.28629900	1.91281700
H	2.87115100	1.02373100	0.78573600
H	2.22240500	2.88082700	-0.60974400
H	0.57115700	4.63144000	-1.18433700
H	-2.36667000	2.60883600	1.16318400
H	-0.72453900	0.85535600	1.72006200
H	-2.71565600	4.55657700	0.01827100
H	1.33571800	0.60307200	-1.68102700
C	-1.37729500	-2.65361400	-0.65022900
C	-0.94096700	-4.08924000	-0.43779300
O	0.20716700	-4.46796500	-0.51174900
O	-1.97930800	-4.87436200	-0.17861000
H	0.19369100	-1.65832900	-1.69706400
H	-2.02501800	-2.62219100	-1.52515300
H	-1.96889300	-2.35723000	0.21345100
H	-1.64942800	-5.79545900	-0.04377100
O	-0.45887500	-7.09455700	0.04651300
H	-0.20826500	-7.51206700	0.87366100
H	0.19887900	-6.40021400	-0.12738100

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explicit-1_ohcarbo.xyz

N	-1.862864	-0.643635	-0.777263
O	-1.842896	-1.307162	1.378932
H	0.058368	-3.364178	-1.985072
C	0.756474	-2.495880	0.749339
C	1.379085	-1.129256	0.761692
C	1.021304	-0.220323	1.755510
C	1.397426	1.108285	1.684916
C	2.118726	1.578199	0.588073
C	2.574421	0.663719	-0.358645
C	2.211181	-0.673014	-0.262667
O	2.394421	2.890186	0.424544
H	-1.002853	-3.487403	-0.012847
H	0.438890	-2.767149	1.754418
H	1.455567	-3.256774	0.399267
H	0.413793	-0.558312	2.582674
H	1.121239	1.795274	2.470755
H	3.185571	1.019388	-1.175293
H	2.583535	-1.369255	-1.004159
H	1.661693	3.402996	0.822350
H	0.637358	-1.853616	-1.751282
C	-2.837983	0.411001	-0.587810
C	-2.267342	1.606935	0.167176
O	-1.888768	1.362870	1.418405
O	-2.176572	2.704667	-0.322701
H	-1.525045	-0.879916	-1.698784
H	-3.690683	0.022016	-0.028018
H	-3.170372	0.758132	-1.559178
H	-1.946178	0.390657	1.607639
O	-0.056643	3.910883	1.282028
H	-0.669582	3.885504	0.533751
H	-0.445281	3.256093	1.871486

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explicit-2_ohcarbo.xyz

N	1.754990	0.044723	-0.406508
O	1.295920	0.410646	1.772105
H	0.232534	3.003296	-1.585671

C	-0.975744	1.969547	0.925846
C	-1.902085	0.876445	0.472769
C	-1.797109	-0.414866	0.988692
C	-2.618285	-1.436412	0.534263
C	-3.566182	-1.182817	-0.452141
C	-3.691722	0.098698	-0.973773
C	-2.865334	1.110740	-0.508783
O	-4.399300	-2.143381	-0.935768
H	0.959149	2.802552	0.519435
H	-0.766302	1.878975	1.989892
H	-1.437602	2.942226	0.755256
H	-1.067576	-0.619562	1.759501
H	-2.529086	-2.430938	0.953038
H	-4.441696	0.288172	-1.727327
H	-2.985514	2.110445	-0.905791
H	-4.229622	-2.975651	-0.484518
H	-0.581556	1.584026	-1.604117
C	2.458669	-1.204659	-0.194601
C	3.814785	-1.049815	0.487874
O	3.797834	-0.442078	1.669570
O	4.828956	-1.477384	-0.000410
H	1.640253	0.432665	-1.331942
H	2.624067	-1.679167	-1.154771
H	1.842037	-1.857438	0.426833
H	2.873790	-0.166624	1.900399
O	6.925841	-0.391128	1.796708
H	6.455447	-0.864701	1.099832
H	6.213402	-0.095878	2.368357

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explicit-3_ohcarbo.xyz

N	-2.005115	-0.575472	-0.788009
O	-2.137993	-1.274361	1.355529
H	0.051838	-3.199523	-1.831401
C	0.650114	-2.088334	0.956045
C	1.420464	-0.832581	0.655808
C	2.634511	-0.887667	-0.021868
C	3.325072	0.270661	-0.360504
C	2.798883	1.511829	-0.024104
C	1.587693	1.592746	0.658641
C	0.917795	0.428389	0.991945
O	3.426701	2.679055	-0.330362
H	-0.926045	-3.310836	0.159160
H	0.217536	-2.053711	1.954575
H	1.317531	-2.949064	0.909136
H	3.060653	-1.849475	-0.277093
H	4.273475	0.206636	-0.879035
H	1.174403	2.556184	0.924208
H	-0.013764	0.506717	1.534637
H	4.254057	2.490905	-0.782990
H	0.782407	-1.760039	-1.547063
C	-3.109036	0.360779	-0.702718
C	-2.792452	1.572273	0.170923
O	-2.555043	1.303785	1.451491
O	-2.773355	2.696103	-0.261665
H	-1.528623	-0.745988	-1.662214
H	-3.983223	-0.145885	-0.288942
H	-3.337886	0.720182	-1.699053
H	-2.531838	0.319310	1.592910

O	-0.758861	3.774036	1.624028
H	-1.133463	3.172120	2.272548
H	-1.402485	3.734196	0.904943

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explicit-4_ohcarbo.xyz

N	-1.873284	-0.691890	-0.634864
O	-1.992018	-1.631756	1.415160
H	0.011564	-3.324358	-2.033595
C	0.781263	-2.443377	0.761166
C	1.322616	-1.043454	0.703765
C	0.809237	-0.070064	1.558992
C	1.108628	1.270450	1.395611
C	1.941433	1.678446	0.352735
C	2.534764	0.711264	-0.456945
C	2.224110	-0.630128	-0.278398
O	2.201830	2.978692	0.109212
H	-0.880413	-3.588632	-0.012108
H	0.475704	-2.691097	1.776226
H	1.525129	-3.173923	0.440780
H	0.142308	-0.366466	2.354910
H	0.684181	2.007585	2.060744
H	3.217388	1.027582	-1.232221
H	2.695470	-1.366774	-0.918031
H	1.502914	3.522538	0.527273
H	0.690845	-1.870666	-1.706777
C	-2.861140	0.336277	-0.379611
C	-2.357486	1.388823	0.605768
O	-2.183433	0.971061	1.846015
O	-2.147791	2.533101	0.274845
H	-1.455331	-0.797053	-1.547614
H	-3.766340	-0.118851	0.026518
H	-3.093180	0.834749	-1.313512
H	-2.259603	-0.018655	1.877752
O	-0.042543	4.208501	1.142533
H	-0.291520	5.109679	0.927901
H	-0.815530	3.657829	0.923078

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explicit-5_ohcarbo.xyz

N	1.778987	0.024840	-0.379550
O	1.335480	0.380241	1.804248
H	0.279812	3.002641	-1.527973
C	-0.943798	1.942170	0.972834
C	-1.874196	0.860431	0.501158
C	-2.848595	1.119515	-0.458285
C	-3.679101	0.113041	-0.937824
C	-3.542434	-1.181658	-0.454067
C	-2.579909	-1.459594	0.512113
C	-1.759365	-0.447852	0.979856
O	-4.321684	-2.213363	-0.877153
H	0.991677	2.777986	0.576543
H	-0.735266	1.832905	2.035351
H	-1.401852	2.919300	0.818227
H	-2.977902	2.128411	-0.828014
H	-4.436521	0.338229	-1.677805
H	-2.495769	-2.467677	0.890604
H	-1.019608	-0.669035	1.736352
H	-4.956323	-1.895160	-1.525991
H	-0.558683	1.597061	-1.558349

C	2.490652	-1.221822	-0.177113
C	3.853533	-1.053529	0.488576
O	3.840804	-0.463215	1.679694
O	4.869543	-1.450570	-0.020697
H	1.661958	0.419734	-1.301683
H	2.648441	-1.693723	-1.139822
H	1.883789	-1.878080	0.449976
H	2.916656	-0.197952	1.921204
O	6.809352	0.362331	1.304458
H	6.457334	-0.357365	0.767249
H	6.136303	0.465380	1.981411

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explicit-6_ohcarbo.xyz

N	1.916160	-0.045752	0.230029
O	1.371970	-1.571923	-1.348395
H	0.006745	-1.588583	2.823571
C	-0.969198	-2.250279	0.167240
C	-1.857421	-1.085093	-0.166196
C	-2.868369	-0.682110	0.701212
C	-3.665854	0.422249	0.422791
C	-3.457251	1.144688	-0.744466
C	-2.455030	0.755773	-1.627311
C	-1.667469	-0.345150	-1.336741
O	-4.204198	2.234373	-1.079940
H	0.905127	-2.722510	1.094751
H	-0.730511	-2.817301	-0.730537
H	-1.482598	-2.916897	0.861472
H	-3.050234	-1.247684	1.605790
H	-4.452414	0.713716	1.107482
H	-2.310220	1.321881	-2.535724
H	-0.889253	-0.643466	-2.024647
H	-4.864574	2.391367	-0.398837
H	-0.539654	-0.345269	1.916262
C	2.931872	0.557160	-0.575457
C	4.232064	-0.216105	-0.536655
O	5.129219	0.308624	-1.414024
O	4.486304	-1.153937	0.160940
H	1.854258	0.137418	1.219168
H	3.131829	1.577932	-0.253447
H	2.601495	0.595603	-1.611995
H	5.935442	-0.222394	-1.340312
O	4.852730	3.174281	-0.884283
H	4.910336	3.858521	-1.553864
H	5.142350	2.360202	-1.310679

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explicit-7_ohcarbo.xyz

N	2.540930	0.260806	0.492701
O	1.945253	1.965274	-0.880215
H	0.776165	-1.665055	-0.933845
C	-0.650050	0.974129	0.515513
C	-2.068699	0.507397	0.356767
C	-2.848922	0.955365	-0.706669
C	-4.146175	0.500137	-0.888751
C	-4.688722	-0.422860	-0.000119
C	-3.928196	-0.881348	1.067572
C	-2.632590	-0.414747	1.236855
O	-5.956602	-0.905292	-0.125819
H	-0.022080	0.491709	-1.475902

H	-0.305468	0.784548	1.533099
H	-0.576716	2.045062	0.329378
H	-2.438457	1.676279	-1.401388
H	-4.739847	0.864931	-1.717529
H	-4.362636	-1.591871	1.755142
H	-2.048700	-0.770067	2.075612
H	-6.376692	-0.506815	-0.893577
H	-0.576237	-1.521656	-0.031058
C	3.909578	0.666151	0.572681
C	4.730597	0.128884	-0.579327
O	5.999001	0.613942	-0.537329
O	4.358753	-0.631088	-1.426352
H	2.260372	-0.663665	0.780493
H	4.367386	0.332030	1.502693
H	3.968455	1.752718	0.544529
H	6.471321	0.232475	-1.291579
O	6.664718	0.310940	2.302051
H	7.151647	0.962679	2.810118
H	6.753140	0.574206	1.379525

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explicit-9_ohcarbo.xyz

N	2.656165	-0.477174	0.907983
O	2.159706	-1.828405	-0.843675
H	0.277744	-1.171744	2.495861
C	-0.279048	-0.045497	-0.588651
C	-1.761368	0.119573	-0.415903
C	-2.298878	1.257906	0.175303
C	-3.669271	1.392678	0.369626
C	-4.526347	0.376794	-0.031490
C	-4.008553	-0.769603	-0.626962
C	-2.642313	-0.888708	-0.812165
O	-5.878041	0.446516	0.126548
H	-0.126765	-1.985757	0.315812
H	0.222461	0.919407	-0.502092
H	-0.048265	-0.450932	-1.572521
H	-1.638899	2.058053	0.482789
H	-4.068833	2.289481	0.826160
H	-4.687520	-1.548256	-0.941879
H	-2.248818	-1.780636	-1.281917
H	-6.109848	1.286637	0.532993
H	-0.806915	-0.110274	1.897967
C	4.020755	-0.312538	0.512479
C	4.179350	0.740114	-0.563400
O	5.463428	0.789989	-1.005344
O	3.323253	1.461206	-0.987539
H	2.231084	0.154590	1.568831
H	4.401636	-1.251853	0.115866
H	4.645391	-0.032544	1.359329
H	5.500077	1.478706	-1.684884
O	6.965014	0.690955	1.509322
H	7.781188	0.201564	1.628937
H	6.795853	0.696290	0.560823

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explicit-11_ohcarbo.xyz

N	-2.644543	0.092197	-0.256052
O	-2.051755	1.922763	0.945017
H	-0.738871	-1.648673	1.227184
C	0.511659	0.914273	-0.495293

C	1.953415	0.512266	-0.371791
C	2.765736	1.073725	0.610621
C	4.087019	0.680686	0.762589
C	4.621812	-0.293310	-0.074791
C	3.829394	-0.864863	-1.061707
C	2.510001	-0.459339	-1.201982
O	5.912066	-0.719298	0.024805
H	-0.002589	0.571559	1.556818
H	0.127179	0.631559	-1.476328
H	0.405082	1.993399	-0.390287
H	2.361403	1.834986	1.264711
H	4.704968	1.133558	1.527723
H	4.257670	-1.614262	-1.710796
H	1.900939	-0.902862	-1.978537
H	6.352629	-0.244042	0.735266
H	0.561258	-1.530425	0.247540
C	-4.029631	0.443119	-0.302345
C	-4.777011	-0.023956	0.927592
O	-6.063785	0.412158	0.906806
O	-4.339079	-0.697013	1.815496
H	-2.341616	-0.841582	-0.484958
H	-4.516165	0.017914	-1.179072
H	-4.128018	1.525678	-0.360039
H	-6.486132	0.080120	1.712312
O	-6.842685	-0.146735	-1.863222
H	-7.379063	0.442022	-2.397660
H	-6.897028	0.189612	-0.962038

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explicit-16_ohcarbo.xyz

N	-2.66302088466181	-0.34570747467823	-0.48966334018246
O	-2.11678719498071	1.65855936435383	-1.38345782402767
H	-1.04677293957343	0.14058873903174	1.86414873132908
C	0.53479569908361	-0.00759903915912	-1.07054894504556
C	1.93572874020962	-0.04961941699824	-0.53133097613641
C	2.49572199232814	-1.23465992513122	-0.06664199530247
C	3.77720088656032	-1.26430146389918	0.47146687341168
C	4.52024330202048	-0.09371503669891	0.54993754088333
C	3.97763419722225	1.10187757066940	0.08815025549011
C	2.70026598635381	1.11502040978013	-0.44361996523994
O	5.78116267156747	-0.05336995787354	1.06173938263282
H	-0.16152459030251	1.56971729878707	0.20562150724438
H	0.21267095471387	-1.01067308058849	-1.35346545833813
H	0.48611621043524	0.62509338901344	-1.95669696279074
H	1.92669962885722	-2.15257728707407	-0.12946267021493
H	4.19830215488732	-2.19756089454163	0.82325919835706
H	4.56929835971915	2.00327920246794	0.14876017617190
H	2.28837533031470	2.04835741953304	-0.80450368748033
H	6.04528844177662	-0.93615309738262	1.33705509334660
H	0.38167584322752	-0.56276071611442	1.44592014676333
C	-4.03825827559694	-0.31367958650596	-0.94473815153088
C	-4.85769596228394	0.68102140614052	-0.12610874125118
O	-4.52684554313306	1.96511315324387	-0.30767923585590
O	-5.71014128459892	0.35180690604834	0.65344426898724
H	-2.36984455524070	-1.00636922827460	0.21643947646018
H	-4.47497809002674	-1.29826614797282	-0.82268217226631
H	-4.05987967615132	-0.03101683894955	-1.99697438531402
H	-3.73518076063670	2.02577260707358	-0.89644364500433
O	-2.98516950054618	1.34205742490150	2.26122863972062

H	-3.78025879480629	0.88456338422634	2.55183555837872
H	-3.32458065990015	2.04945637039697	1.70214608103450

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explicit-17_ohcarbo.xyz

N	2.928688	-0.148671	-0.982454
O	2.274693	1.841754	-0.148952
H	-0.325950	-1.646876	-0.725325
C	-0.254605	0.838252	0.558435
C	-1.692732	0.414595	0.500477
C	-2.179642	-0.602893	1.314227
C	-3.500316	-1.027693	1.228207
C	-4.359625	-0.432521	0.313554
C	-3.893289	0.587757	-0.508907
C	-2.574770	0.999213	-0.409531
O	-5.665107	-0.800188	0.180760
H	0.143537	0.475402	-1.521069
H	0.186692	0.556659	1.514830
H	-0.164877	1.918663	0.460133
H	-1.520066	-1.065325	2.036209
H	-3.862235	-1.815892	1.876417
H	-4.574146	1.049093	-1.208926
H	-2.224169	1.800490	-1.047284
H	-5.867195	-1.497538	0.811287
H	0.850978	-1.577648	0.412852
C	4.340055	0.176359	-0.973155
C	4.917657	0.151127	0.439236
O	4.334928	1.010169	1.295107
O	5.798196	-0.583364	0.785589
H	2.611290	-1.091694	-1.155599
H	4.479338	1.171405	-1.397288
H	4.877542	-0.550163	-1.571634
H	3.649833	1.544669	0.820006
O	2.260376	-0.947101	2.167281
H	2.619618	-1.636619	2.730927
H	2.940637	-0.260338	2.156136

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explicit-4b_ohcarbo.xyz

N	0.77943673590224	2.02638734491795	1.17107996080189
O	0.62159877600994	2.33494608434897	-1.05946629953680
H	3.33521207637402	-0.40428069389602	1.00802000435322
C	1.67948324274834	-0.32041503727681	-1.44338609737769
C	0.55197445238014	-1.23664151263276	-1.05659289568145
C	0.78874111529583	-2.57770400097092	-0.75609463957410
C	-0.23073695064868	-3.42062584901337	-0.33765838834160
C	-1.51971412534664	-2.92040967383368	-0.20475774575948
C	-1.77670787932507	-1.58556900853581	-0.49727714807797
C	-0.75001001147928	-0.75711547662082	-0.92233064490485
O	-2.49095605081216	-3.77959557057470	0.21515228488186
H	3.01809047450191	1.12266892332128	-0.59254396432547
H	1.40079160264985	0.30693678386451	-2.28835267819554
H	2.54628826885642	-0.91337970722441	-1.73678883313595
H	1.79016645096980	-2.97493362101663	-0.86026944048184
H	-0.04352349969016	-4.46052109026591	-0.11407274301208
H	-2.77629978233457	-1.18615847413435	-0.38296625394228
H	-0.96668588793844	0.27777367201368	-1.13966148807696
H	-3.32891231491856	-3.31035365187806	0.26542474553477
H	1.77683188765454	-0.88733913021007	1.07057948171453
C	-0.14558236473932	3.07934570629030	1.47557325285357

C	-1.56072355892834	2.74823331185860	1.04323724698943
O	-2.01266463503701	1.65121152639591	0.87230685114021
O	-2.28772164387512	3.87739822880697	0.90261758095111
H	1.19616474873611	1.44437280271418	1.88043189458651
H	0.15107243467819	4.01209128752237	0.99953568893117
H	-0.16346280045431	3.24120266865716	2.55242917923357
H	-3.19069155818669	3.60676170252782	0.68097971675801
O	-0.10629504289746	5.11378295423687	-1.12264334482770
H	0.13152346661734	4.18320459383473	-1.25424802545955
H	-1.01736262104469	5.08976886079315	-0.82038914407013

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explicit-4c-ohcarbo.xyz

N	-0.231294	-1.833526	-0.545598
O	0.351027	-1.445312	1.604767
H	2.575346	-0.119217	-1.941438
C	1.927009	0.790817	0.737588
C	0.843623	1.803514	0.495630
C	1.021851	2.843623	-0.416361
C	0.013675	3.757625	-0.686376
C	-1.207057	3.641487	-0.034696
C	-1.404782	2.615186	0.882892
C	-0.388367	1.707337	1.142048
O	-2.169580	4.561355	-0.326789
H	2.606271	-1.131984	0.074678
H	1.948999	0.497543	1.785406
H	2.896727	1.223109	0.487250
H	1.975466	2.950786	-0.916903
H	0.160765	4.565329	-1.388100
H	-2.353555	2.528244	1.397709
H	-0.549459	0.910211	1.853615
H	-2.957440	4.373411	0.191572
H	1.102839	0.557551	-1.743001
C	-1.255418	-2.766638	-0.191965
C	-0.698502	-4.135279	0.134385
O	0.431638	-4.500889	-0.008482
O	-1.674809	-4.950127	0.617272
H	0.108851	-1.760739	-1.491469
H	-1.976580	-2.873834	-1.000490
H	-1.792387	-2.410219	0.685117
H	-1.254271	-5.799201	0.816129
O	-3.860862	-4.301911	-1.231024
H	-4.517830	-4.921330	-1.553860
H	-3.394339	-4.753461	-0.519186